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	NEWS		JAN	12	Match STN Content and Features to Your Information
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	NEWS	3	JAN	25	Annual Reload of MEDLINE database
	NEWS	4	FEB	16	STN Express Maintenance Release, Version 8.4.2, Is
					Now Available for Download
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					of Author Abstracts
	NEWS		FEB		New FASTA Display Formats Added to USGENE and PCTGEN
	NEWS	7	FEB	16	INPADOCDB and INPAFAMDB Enriched with New Content
		_			and Features
	NEWS	8	FEB	Τ6	INSPEC Adding Its Own IPC codes and Author's E-mail
	NEWS	9	APR	0.2	CAS Registry Number Crossover Limits Increased to
	NEWS	9	APR	02	500,000 in Key STN Databases
	NEWS	10	APR	0.2	PATDPAFULL: Application and priority number formats
	MEND	10	TIL IX	02	enhanced
	NEWS	11	APR	0.2	
	NEWS		APR		New Thesaurus Added to Derwent Databases for Smooth
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					Coverage back to 1948
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	NEWS	EXP	RESS		RUARY 15 10 CURRENT WINDOWS VERSION IS V8.4.2, CURRENT DISCOVER FILE IS DATED 15 JANUARY 2010.
				MND	CORRENT DISCOVER FILE IS DATED IS JANUARY 2010.
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FULL ESTIMATED COST

SINCE FILE TOTAL ENTRY SESSION 0.22

0.22

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STRUCTURE FILE UPDATES: 26 APR 2010 HIGHEST RN 1220389-58-1 DICTIONARY FILE UPDATES: 26 APR 2010 HIGHEST RN 1220389-58-1

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http://www.cas.org/support/stngen/stndoc/properties.html

Uploading C:\Program Files\Stnexp\Oueries\10591884.str

chain nodes : 11 12

ring nodes :

1 2 3 4 5 6 7 8 9 10

ring bonds :

 $1-2 \quad 1-6 \quad 2-3 \quad 2-12 \quad 3-4 \quad 3-11 \quad 4-5 \quad 5-6 \quad 5-7 \quad 6-10 \quad 7-8 \quad 8-9 \quad 9-10$ exact/norm bonds :

1-2 1-6 2-3 2-12 3-4 3-11 4-5 5-6 5-7 6-10 7-8 8-9 9-10

G1:C,N

L1

Match level :

1:CLASS 2:CLASS 3:CLASS 4:CLASS 5:CLASS 6:CLASS 7:CLASS 8:CLASS 9:CLASS 10:CLASS 11:CLASS 12:CLASS

#### L1 STRUCTURE UPLOADED

STR

=> d l1 L1 HAS NO ANSWERS



Structure attributes must be viewed using STN Express query preparation.

=> 8 11

SAMPLE SEARCH INITIATED 15:57:15 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 100686 TO ITERATE

2.0% PROCESSED 2000 ITERATIONS INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED) 16 ANSWERS

INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*INCOMPLETE\*\*
BATCH \*\*COMPLETE\*\*

PROJECTED ITERATIONS: 1994848 TO 2032592 PROJECTED ANSWERS: 14407 TO 17811

L2 16 SEA SSS SAM L1

=> file caplus

 COST IN U.S. DOLLARS
 SINCE FILE
 TOTAL

 ENTRY
 SESSION

 FULL ESTIMATED COST
 2.45
 2.67

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FILE COVERS 1907 - 28 Apr 2010 VOL 152 ISS 18
FILE LAST UPDATED: 27 Apr 2010 (20100427/ED)
REVISED CLASS FIELDS (/NCL) LAST RELOADED: Feb 2010
USPTO MANUAL OF CLASSIFICATIONS THESAURUS ISSUE DATE: Feb 2010

CAplus now includes complete International Patent Classification (IPC) reclassification data for the first quarter of 2010.

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# http://www.cas.org/legal/infopolicy.html

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s 12 L3

18 L2

=> d abs fbib 15-18

3 ANSWER 15 OF 18 CAPLUS COPYRIGHT 2010 ACS on STN

AB In order to obtain antitumor agents, various 7H-pyridocarbazole dimers were prepared by quaternization of the pyridinic N atoms of the different isomeric 7H-pyridocarbazole rings with haloamino alicyclic or aliphatic chains. The dimers interact with DNA more markedly than the corresponding monomers, and the bisintercalation depends upon the nature, flexibility and ionization state of the linking chains. They most often bisintercalate at pH 5, where the chain is protonated, and monointercalate at pH 7.4. The apparent binding consts. (Kap) were 108-109 M-1 at pH 5 and (5 + 105)-(2 + 107) M-1 at pH 7.4. The bisintercalating dimers covered 4 DNA base pairs, whereas most of the monointercalating dimers covered 2 bases pairs. The antitumor activity against L1210 murine leukemia is strongly dependent on the position of attachment and the nature and rigidity of the linking chain. Three highly active dimers were obtained among 7H-pyrido[4,3-c]carbazole dimers with rigid bis(thylpiperidinyl) chains. On the other hand, 2 ellipticine dimers were prepared which were completely inactive against L1210.

AN 1980:604501 CAPLUS Full-text

DN 93:204501

OREF 93:32629a

- TI DNA intercalating compounds as potential antitumor agents. 2. Preparation and properties of 7H-pyridocarbazole dimers
- AU Pelaprat, Didier; Delbarre, Alain; Guen, Irene Le; Le Pecq, Jean Bernard; Roques, Bernard P.
- CS Dep. Chim. Org., Unites Enseign. Rech. Sci. Pharm. Biol., Paris, 75006, Fr.
- SO Journal of Medicinal Chemistry (1980), 23(12), 1336-43 CODEN: JMCMAR: ISSN: 0022-2623
- DT Journal
- LA English

OSC.G 23 THERE ARE 23 CAPLUS RECORDS THAT CITE THIS RECORD (23 CITINGS)

L3 ANSWER 16 OF 18 CAPLUS COPYRIGHT 2010 ACS on STN

- AB Structural studies on the six alkaloids isolated from T. crebriflora are described. Spectral data indicate that five of these alkaloids (A-E) posses the dibenzo[f,h]pyrrolo[1,2-b]isoquinoline skeleton present in tylocrebine. They differ in the number, nature, and distribution of the O-bearing substituents and in the presence or absence of a benzylic-type hydroxyl.
- AN 1971:13314 CAPLUS Full-text
- DN 74:13314
- OREF 74:2149a,2152a
- TI Alkaloids of Tylophora. II. Structural studies
- AU Rao, Koppaka Visweswara CS John L. Smith Mem. Cancer Res., Chas. Pfizer and Co., Inc., Maywood, NJ, HSA
- SO Journal of Pharmaceutical Sciences (1970), 59(11), 1608-11 CODEN: JPMSAE; ISSN: 0022-3549
- DT Journal
- LA English
- OSC.G 2 THERE ARE 2 CAPLUS RECORDS THAT CITE THIS RECORD (2 CITINGS)
- L3 ANSWER 17 OF 18 CAPLUS COPYRIGHT 2010 ACS on STN
- AB Irradiation of solns. of thebainequinone (I)or thebainehydroquinone (II) in dioxane under N, using a high-pressure Hg lamp, gave photochebainehydroquinone (III), m. 156-7°. The mechanism was believed to involve intramol. sensitization of the C7-C8 double bond in I and II by the enedione or the hydroquinone system. The photochem. interconversion of I and II was suggested by the observation that each could give III.
- AN 1965:51868 CAPLUS Full-text
- DN 62:51868
- OREF 62:9185b-d
- TI Isolation and structure of photothebainehydroquinone
- AU Barneis, Z. J.; Wheeler, D. M. S.; Kinstle, T. H.
- CS Univ. of Nebraska, Lincoln
- SO Tetrahedron Letters (1965), (4), 275-80 CODEN: TELEAY; ISSN: 0040-4039
- DT Journal
- LA English
- L3 ANSWER 18 OF 18 CAPLUS COPYRIGHT 2010 ACS on STN
- AB Vat dyes or intermediates are prepd. by the treatment with alk. condensing agents of Bz-2-, -3-, -4-, -6- or -7-azabenzanthrones or homologs or derivs. thereof that are not substituted in either of the peri-positions or are only substituted therein by substituents that are readily split off or that may be connected in a peri-position with an aromatic radical containing at least 2 condensed rings by means of a N bridge. Starting materials having 2 reactive peri-positions (materials wherein 1 peri-position contains a substituent that is easily displaced being included) yield by the above treatment carried out below 100° diazabenzanthronyls but by treatment at higher temps., when a periposition is occupied by a pyrazolanthrone or anthraquinone or other vattable radical, condensation products containing an acridine ring are obtained. Bz-2-Azabenzanthrones are obtained by condensing anthraquinone-1-carboxylic acid chloride (I) with aminoacetic acid esters, treating the resulting compound with alc., saponifying the resulting ester and splitting off CO2. Bz-3azabenzanthrones are prepared by treating 4-benzoylisoquinolines having a reactive 5-position with a condensing agent of the AlCl3 type. Bz-4-Azabenzanthrones are similarly derived from 1-benzoylisoquinolines having a reactive 8-position. Bz-6- and Bz-7-azabenzanthrones are obtained from  $\beta$ anthraquinones or the corresponding reduction products by treatment with glycerol in the presence of H2SO4. Among examples, (1) the azabenzanthrone obtained by treating 2-azanthraquinone with qlycerol and H2SO4is condensed with alc. KOH at 140-145°; the product dyes vegetable fibers violet shades, (2) Bz-1-hydroxy-Bz-2-azabenzanthrone, prepared by condensing I with

aminoacetic acid Et ester, splitting off H2O, saponifying and decarboxylating, is treated with KOH at 215–222°; the product dyes blue-green shades, (3) the condensation products of Bz-l-bromodimethyl-6-azabenzanthrone and 1-aminoanthraquinone (II) or pyrazolanthrone or the condensation product of a dibrominated derivative of dimethylazabenzanthrone and II are condensed with alc. KOH at about 140° (olive-green, blue and gray shades, resp.).

AN 1936:65004 CAPLUS Full-text

DN 30:65004

OREF 30:8638b-g

TI Vat dyes; intermediates

PA I. G. Farbenindustrie A.-G.

SO Addn. to 421,264 (C. A. 29, 3531.3)

DT Patent

LA Unavailable

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE		
PI	GB 450244		19360710	GB 1934-35445	19341210		

=> file registry

COST IN U.S. DOLLARS SINCE FILE TOTAL

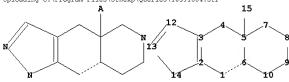
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### http://www.cas.org/support/stngen/stndoc/properties.html

= 3

Uploading C:\Program Files\Stnexp\Queries\10591884.str



chain nodes :

15

ring nodes :

1 2 3 4 5 6 7 8 9 10 12 13 14

chain bonds : 5-15

ring bonds :

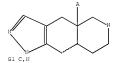
1-2 1-6 2-3 2-14 3-4 3-12 4-5 5-6 5-7 6-10 7-8 8-9 9-10 12-13 13-14 exact/norm bonds:

13-14 3-4 3-12 4-5 5-6 5-7 5-15 6-10 7-8 8-9 9-10 12-13 13-14

Match level: 1:CLASS 2:CLASS 3:CLASS 4:CLASS 5:CLASS 6:CLASS 7:CLASS 8:CLASS 9:CLASS 10:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS

#### L4 STRUCTURE UPLOADED

=> d 14 L4 HAS NO ANSWERS L4 STR



Structure attributes must be viewed using STN Express query preparation.

=> s 14 SAMPLE SEARCH INITIATED 16:02:37 FILE 'REGISTRY' SAMPLE SCREEN SEARCH COMPLETED - 6746 TO ITERATE

29.6% PROCESSED 2000 ITERATIONS INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED) SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*
BATCH \*\*COMPLETE\*\*

PROJECTED ITERATIONS: 129995 TO 139845 PROJECTED ANSWERS: 12 TO 392

L5 3 SEA SSS SAM L4

=> s 14 ful

FULL SEARCH INITIATED 16:02:51 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 132774 TO ITERATE

100.0% PROCESSED 132774 ITERATIONS

215 ANSWERS

3 ANSWERS

SEARCH TIME: 00.00.04

L6 215 SEA SSS FUL L4

=> file caplus

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This file contains CAS Registry Numbers for easy and accurate

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=> s 16
L7 15 L6
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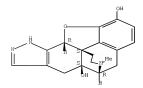
=> d abs fbib hitstr 10-15

- L7 ANSWER 10 OF 15 CAPLUS COPYRIGHT 2010 ACS on STN
- AB Oxymorphazole (17-methyl-6,7-dehydro-3,14-dihydroxy-4,5\alpha-epoxy-6,7:3',4'pyrazolomorphinan), a hydrophilic opioid, given intracerebroventricularly (2.5-50 nmol) or intrathecally (0.3-5 nmol) dose-dependently produced tailflick inhibition in male CD-1 mice. However, oxymorphazole given s.c. even at high doses (10-80 mg/kg) produced weak tail-flick inhibition. Oxymorphazole given i.p. (0.1 to 10 mg/kg) dose-dependently inhibited abdominal constriction response induced by i.p. injection of 0.6% acetic acid. Oxymorphazole given intracerebroventricularly (25 nmol) or intrathecally (5 nmol) induced tailflick inhibition was blocked by pretreatment with the u-opioid receptor antagonist D-Phe-Cys-Tyr-D-Orn-Thr-Pen-Thr-NH2, but not κ-opioid receptor antagonist nor-binaltorphimine. The  $\delta$ -opioid receptor antagonist, naltrindole, blocked the tail-flick inhibition induced by oxymorphazole given intrathecally but not intracerebroventricularly. The inhibition of the abdominal constriction response by oxymorphazole given i.p. was blocked by i.p. pretreatment with naloxone, but not naltrindole or nor-binaltorphimine. Thus, oxymorphazole given systemically produces antinociception only with the abdominal constriction test, but not the tail-flick test, suggesting that it produces the antinociception at the peripheral sites when administered systemically. The oxymorphazole-induced antinociception is mainly mediated by the stimulation of  $\mu$ -opioid receptors when given either centrally or systemically and also the  $\delta$ -opioid receptors when given intrathecally. The lack of central antinociceptive effect of oxymorphazole given systemically may have interesting clin. implications.

AN 2003:581379 CAPLUS Full-text

DN 140:87492

- TI Antinociceptive properties of oxymorphazole in the mouse
- AU Wu, Hsiang-en; Sun, Han-Sen; Darpolar, Moses; Dunn, William; Tseng, Leon F.
- CS Department of Anesthesiology, Medical College of Wisconsin, Milwaukee, WI, 53226, USA
- SO European Journal of Pharmacology (2003), 473(2-3), 143-148 CODEN: EJPHAZ; ISSN: 0014-2999
- PB Elsevier Science B.V.
- DT Journal
- LA English
- IT 644996-43-0
  - RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
- (antinociceptive properties of oxymorphazole in the mouse)
- RN 644996-43-0 CAPLUS
- CN 5,10c-(Iminoethano)-10cH-furo[2',3',4',5':4,5]phenanthro[3,2-c]pyrazole-1,5a(6H)-diol, 4,5,9,9b-tetrahydro-13-methyl-, dihydrochloride, (5R,5aS,9bR,10cS)- (9CI) (CA INDEX NAME)



2 HC1

OSC. G. THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD (1 CITINGS) RE.CNT 19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

ANSWER 11 OF 15 CAPLUS COPYRIGHT 2010 ACS on STN

- In an effort to establish the importance of the N-(2-methylallyl) substituent AR in the noroxymorphone series, several derivs., e.g. I, were synthesized, retaining that N-substituent and modifying the  $\delta$  address moiety. A few compds. showed moderate binding affinity and selectivity for the  $\delta$  receptor; none displayed a pharmacol. profile as exceptional as N-(2methylallyl)noroxymorphindole. A second study showed that 3-0-methylation of all derivs. decreases binding affinity. The present results indicate that only a combination of the N-(2-methylallyl) group and an indole  $\delta$  address provided high selectivity for the  $\delta$  receptor. AN
- 2001:746618 CAPLUS Full-text
- DM 136:69989
- тт Derivatives of 17-(2-methylallyl)-substituted noroxymorphone: variation of the delta address and its effects on affinity and selectivity for the delta opioid receptor
- Ullrich, T.; Dersch, C. M.; Rothman, R. B.; Jacobson, A. E.; Rice, K. C. AU
- CS Laboratory of Medicinal Chemistry, NIDDK, National Institutes of Health, Bethesda, MD, 20892, USA
- SO Bioorganic & Medicinal Chemistry Letters (2001), 11(21), 2883-2885 CODEN: BMCLE8; ISSN: 0960-894X
- PR Elsevier Science Ltd.
- Journal DT
- LA English
- OS CASREACT 136:69989

### IT 384820-59-1P

CN

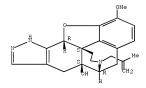
RL: DMA (Drug mechanism of action); PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent)

(preparation of 17-(2-methylallyl)-substituted noroxymorphone derivs. variation of delta address and effects on affinity and selectivity for delta opioid receptor)

RN 384820-59-1 CAPLUS

5,10c-(Iminoethano)-10cH-furo[2',3',4',5':4,5]phenanthro[3,2-c]pyrazol-5a(6H)-ol, 4,5,9,9b-tetrahydro-1-methoxy-13-(2-methyl-2-propenyl)-, (5R,5aS,9bR,10c5)- (9CI) (CA INDEX NAME)

# Absolute stereochemistry.



### IT 384820-63-7P

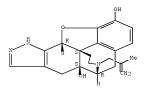
CN

RL: DMA (Drug mechanism of action); PAC (Pharmacological activity); SFN (Synthetic preparation); BIOL (Biological study); PREP (Preparation) (preparation of 17-(2-methylallyl)-substituted noroxymorphone derivs. variation of delta address and effects on affinity and selectivity for delta opioid receptor)

RN 384820-63-7 CAPLUS

5,10c-(Iminoethano)-10cH-furo[2',3',4',5':4,5]phenanthro[3,2-c]pyrazole-1,5a(6H)-diol, 4,5,9,9b-tetrahydro-13-(2-methyl-2-propenyl)-,(5R,5a5,9bR,10c5)-(9CI) (CA INDEX NAME)

#### Absolute stereochemistry.



OSC.G 5 THERE ARE 5 CAPLUS RECORDS THAT CITE THIS RECORD (5 CITINGS)
RE.CNI 19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

AB The compds. I and II [R1 = H, C1-6-alkyl, C2-6-alkenyl, C1-3-alkylenearyl, C3-8-cvcloalkvl, C1-3-alkvlene-C3-8-cvcloalkvl, C1-3-alkvlene-C3-8heterocycloalkyl, C3-8-heterocycloalkyl, aryl, aryl-C1-3-alkyl; R2 = halo, CF3, C1-6-alkvl, C3-8-cvcloalkvl, C(:0)ORa, ORa, C1-3-alkvlene-C3-8cycloalkyl; R3 = H, C1-6-alkyl, C2-6-alkenyl, C2-6-alkynyl; Ra = H, C1-6alkyl, C3-8-cycloalkyl, C1-4-alkylene-C(:0)ORb, aryl, aryl-C1-3-alkyl, C1-3alkenylaryl, Het; Rb = H, C1-6-alkyl, aryl, aryl, aryl-C1-3-alkyl, C1-3alkenylaryl, Het; Het = 5 to 6 membered heterocycle, saturated, or partially or fully unsatd., containing at least one of O, N, S, optionally substituted with C1-6-alkyl; n = 0 - 2] and their pharmaceutically acceptable salts and hydrates and their use as therapeutic agents is disclosed. Thus, I (R1 = R2 = H, R3 = Me) and II (R1 = R2 = H, R3 = Me) were prepared from oxymorphone via regioselective O-methylation with Me3SiCHN2 in MeOH/MeCN, condensation with Me2NCHO in Me2NCOMe, cyclocondensation with hydrazine hydrate in aqueous MeOH and O-deprotection with BBr3 in CH2Cl2. Compound I or II is an agonist for the  $\mu$  and  $\delta$  opioid receptors, and antagonist for the  $\kappa$  opioid receptor, and has high affinity at all three receptors; compound I or II has utility in a variety of therapeutic and research areas where κ opioid receptor antagonism is beneficial, including the treatment of opiate addiction or pain, or in a method of stimulating an immune system of a human. Thus, I (R1 = R2 = H, R3 = Me) and II (R1 = R2 = H, R3 = Me) have high affinity for opioid receptors: Ki (SEM) = 3.75 (0.71) nM vs. μ opioid receptor ([3H]-DAMGO); Ki (SEM) = 19.06 (1.17) vs.  $\delta$  opioid receptor ([3H]-Cl-DPDPE); Ki (SEM) = 12.29 (6.20) nM vs.  $\kappa$ opioid receptor ([3H]-U69,593).

AN 2001:472723 CAPLUS Full-text

DN 135:61469

ΤI Preparation of nonpeptide kappa opioid receptor antagonists

IN Dunn, William; Bauer, Ludwig; Bhargava, Hemendra N.

PA Board of Trustees of the University of Illinois, USA

SO PCT Int. Appl., 25 pp.

CODEN: PIXXD2

DT Patent

LA.

English FAN.CNT 1

	PATENT NO.					KIN	D	DATE			APPL	ICAT	TON .	NO.		D.	ATE	
							-									-		
PΙ	WO 2001046198				A2		20010628			WO 2	20001130							
	WO 2001046198					А3		2002	0510									
		W:	ΑE,	AG,	AL,	AM,	ΑT,	AU,	AZ,	BA,	BB,	BG,	BR,	BY,	BZ,	CA,	CH,	CN,
			CR	CII	CZ.	DE	DK	DM	DZ.	EE	ES	FT	GB	GD	GE	GH	GM	HR

CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT,

LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA. ZW RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG A 19991203

US 1999-454670

US 6284769 В1 20010904 US 1999-454670 19991203 ASSIGNMENT HISTORY FOR US PATENT AVAILABLE IN LSUS DISPLAY FORMAT

CASREACT 135:61469; MARPAT 135:61469

259173-73-4P IΤ

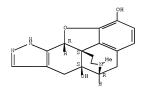
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(preparation of nonpeptide kappa opioid receptor antagonists and mu and delta opioid receptor agonists)

RM 259173-73-4 CAPLUS

CN 5,10c-(Iminoethano)-10cH-furo[2',3',4',5':4,5]phenanthro[3,2-c]pyrazole-1,5a(6H)-diol, 4,5,9,9b-tetrahydro-13-methyl-, (5R,5aS,9bR,10cS)- (9CI) (CA INDEX NAME)

### Absolute stereochemistry.



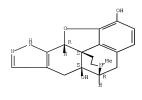
345238-02-0P IΤ

> RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses) (preparation of nonpeptide kappa opioid receptor antagonists and mu and

delta opioid receptor agonists)

RN 345238-02-0 CAPLUS

5,10c-(Iminoethano)-10cH-furo[2',3',4',5':4,5]phenanthro[3,2-c]pyrazol-CN 1,5a(6H)-diol, 4,5,9,9b-tetrahydro-13-methyl-, monohydrochloride, (5R, 5aS, 9bR, 10cS) - (9CI) (CA INDEX NAME)



HC1

7096-91-5P

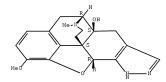
IT

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of nonpeptide kappa opioid receptor antagonists and mu and delta opioid receptor agonists)

RN 7096-91-5 CAPLUS

CN 5,10c-(Iminoethano)-10cH-furo[2',3',4',5':4,5]phenanthro[3,2-c]pyrazol-5a(6H)-ol, 4,5,9,9b-tetrahydro-1-methoxy-13-methyl-, (5R,5aS,9bR,10cS)-(9CI) (CA INDEX NAME)



- osc.G THERE ARE 5 CAPLUS RECORDS THAT CITE THIS RECORD (5 CITINGS) THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD RE.CNT 2 ALL CITATIONS AVAILABLE IN THE RE FORMAT
- L7 ANSWER 13 OF 15 CAPLUS COPYRIGHT 2010 ACS on STN GI

- AB A class of opioid receptor-active derivs. of naltrexone has been synthesized using a common enaminone intermediate. The intermediate used in the synthesis is prepared from DMF di-Me acetal and naltrexone and can be isolated and characterized. The derivs. [I; R = H, Me, Ph, NH2] have heterocyclic groups fused to the 6,7-positions of the morphian system and all were synthesized in 82-100% yield. All compds. were very high affinity, nonselective antagonists for the opioid receptors.
- AN 2000:27207 CAPLUS Full-text
- DN 132:194534
- TI Synthesis and opioid receptor binding properties of 17-cyclopropylmethyl-6,7-dehydro-3,14-dihydroxy-4,50-epoxy-6,7:4',5'-pyrimidinomorphinans
- AU Xu, Wei; Huang, Liang-Fu; Bauer, Ludwig; Bhargava, Hemendra N.; Dunn, William J., III
- CS College of Pharmacy, University of Illinois at Chicago, Chicago, IL, 60612-7231, USA
- SO Medicinal Chemistry Research (1999), 9(6), 389-407 CODEN: MCREEB: ISSN: 1054-2523
- PB Birkhaeuser Boston
- DT Journal
- LA English
- OS CASREACT 132:194534
- IT 259827-05-9P 259827-11-7P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

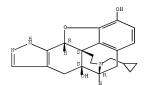
(synthesis and opioid receptor binding properties of

17-cyclopropylmethyl-6,7-dehydro-3,14-dihydroxy-4,5α-epoxy-

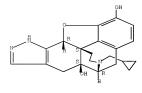
6,7:4',5' -pyrimidinomorphinans)

- RN 259827-05-9 CAPLUS
- CN 5,10c-(Iminoethano)-10cH-furo[2',3',4',5':4,5]phenanthro[3,2-c]pyrazole-1,5a(6H)-diol, 13-(cyclopropylmethyl)-4,5,9,9b-tetrahydro-, (SR,5a5,9bR,10cS)- (9GI) (CA INDEX NAME)

Absolute stereochemistry.



- RN 259827-11-7 CAPLUS
- CN 5,10c-(Iminoethano)-10cH-furo[2',3',4',5':4,5]phenanthro[3,2-c]pyrazole-1,5a(6H)-diol, 13-(cyclopropylmethyl)-4,5,9,9b-tetrahydro-, dihydrochloride, (5R,5a5,9bR,10c5)- (9CI) (CA INDEX NAME)



2 HC1

TT 259827-18-4P

> RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

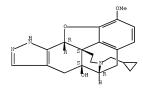
(synthesis and opioid receptor binding properties of

17-cvclopropvlmethyl-6,7-dehydro-3,14-dihydroxy-4,5α-epoxy-6,7:4',5' -pyrimidinomorphinans)

RN

259827-18-4 CAPLUS

CN 5,10c-(Iminoethano)-10cH-furo[2',3',4',5':4,5]phenanthro[3,2-c]pyrazol-5a(6H)-ol, 13-(cyclopropylmethyl)-4,5,9,9b-tetrahydro-1-methoxy-, (5R, 5aS, 9bR, 10cS) - (9CI) (CA INDEX NAME)



- OSC. G 3 THERE ARE 3 CAPLUS RECORDS THAT CITE THIS RECORD (3 CITINGS) RE.CNT 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT
- L7 ANSWER 14 OF 15 CAPLUS COPYRIGHT 2010 ACS on STN
- AΒ A class of opioid receptor active derivs, of oxymorphone was synthesized using a common enaminone intermediate. The derivs. have pyrimidino or pyrazolo rings fused to the 6,7-positions of the morphinan system and all were synthesized in high yield. A pyrazolo derivative is an agonist for the  $\boldsymbol{\mu}$  and  $\delta$  receptors and an antagonist for the  $\kappa$  receptor.
- 1999:810829 CAPLUS Full-text AN
- DN 132:180743
- TI Synthesis and opiate receptor binding properties of 17-methy1-6,7-dehydro-3,14-dihydroxy-4,5α-epoxy-6,7:4',5'-

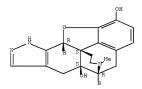
pyrimidinomorphinans

- AU Xu, Wei; Huang, Liang-Fu; Bauer, Ludwig; Bhargava, Hemendra N.; Dunn, William J., III
  CS College of Pharmacy, University of Illinois at Chicago, Chicago, IL,
- 60612-7231, USA
- SO Bioorganic & Medicinal Chemistry Letters (1999), 9(23), 3375-3380 CODEN: BMCLE8; ISSN: 0960-894X
- PB Elsevier Science Ltd.
- DT Journal
- LA English
- IT 259173-73-4P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(preparation and opiate receptor binding of dehydrohydroxyepoxypyazolomorphinan)

- RN 259173-73-4 CAPLUS
- CN 5,10c-(Iminoethano)-10cH-furo[2',3',4',5':4,5]phenanthro[3,2-c]pyrazole-1,5a(6H)-dio1, 4,5,9,9b-tetrahydro-13-methyl-, (5R,5aS,9bR,10cS)- (9CI) (CA INDEX NAME)



- OSC.G 6 THERE ARE 6 CAPLUS RECORDS THAT CITE THIS RECORD (6 CITINGS)
  RE.CNT 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS RECORD
  ALL CITATIONS AVAILABLE IN THE RE FORMAT
- L7 ANSWER 15 OF 15 CAPLUS COPYRIGHT 2010 ACS on STN
- GI For diagram(s), see printed CA Issue.
- AB A soln. of 12 g. 14-hydroxydihydrocodeinone (I) and 8 g. p-MeC6H4SO3H in 40 ml. McOH was adjusted to pH 2 with p-MeC6H4SO3H, treated with 12 ml. trimethyl orthoformate, refluxed 2 hrs., poured into N NaOH, and filtered. The precipitate was washed with 500 ml. ether to give 14-hydroxy-6-methoxy-Δ6.7dihydrodeoxycodeine (II), m. 196-7°, [a]D -228°. The ether solution gave 6,6dimethoxy-14-hydroxydihydrodeoxycodeine (III), m. 121-2°, [a]D-179°. Similarly were prepared 6-ethoxy-14hydroxy-A6.7-dihydrodeoxycodeine, m. 182-4°, [α]D -231°, and 6-butoxy-14-hydroxy-Δ6.7- dihydrodeoxycodeine, m. 121-2°,  $[\alpha]$ D -228°. Enol ethers of higher alcs, were slightly more difficult to prepare A mixture of 1 g. I, 0.66 g. p-MeC6H4SO3H, 5 ml. tricvclohexvl orthoformate, and a trace of cyclohexanol was heated under reflux in toluene 4 hrs. with azeotropic distillation of H2O to give 65% 6-cyclohexyloxy-14hydroxy- $\Delta 6.7$ - dihydrodeoxycodeine, m. 160.5-1.5°, [ $\alpha$ ]D -220°. Similarly a mixture of 9 q. I, 4 ml. morpholine, and 3 q. p-MeC6H4SO3H in 100 ml. PhMe was heated 2 hrs. with azeotropic distillation of H2O to give 9.2 g. 14-hydroxy-6-

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morpholino-\Delta 6.7 -dihydrodeoxycodeine, m. 201-2°, [\alpha]D -282°. Similarly were
prepared 14-hydroxy-6-pyrrolidino-\Delta 6.7-dihydrodeoxycodeine, m. 190-1°, [\alpha]D -
300°, and 14-hydroxy-6-methylanilino-Δ6.7- dihydrodeoxycodeine, m. 195-6°,
[\alpha]D -58°. The Vilsmeier reaction was carried out by adding a solution of the
alkaloid in 1,2-dichloroethane to the Vilsmeier reagent prepared from POC13
and dimethylformamide in the same solvent at 0°. The mixture was heated at
appropriate temperature and finally hydrolyzed in aqueous solution buffered to
the required pH. Thus a mixture of 12 q. II and III in 100 ml. 1,2-
dichloroethane and a mixture of 20 ml. dimethylformamide and 12 mh POCl3 in 20
ml. 1,2-dichloroethane was heated at 65-70° 7 hrs., added to 40 g. Na2HPO4 in
1 h H2O, pH adjusted to between 8 and 9.5 with 2N NaOH, and the mixture
stirred 30 min. and extracted with CHCl3 to give a product which contained
about 20% 6-chloro-7-formyl-14-hydroxy-\Delta6.7- dihydrodeoxycodeine (IV). This
substance was refluxed in MeOH solution with NaOAc 6 hrs. to give 6.5 g. 7-
formyl-14-hydroxy-6-methoxy-Δ6.7- dihydrodeoxycodeine (V), m. 185-6°. The
residue from the mother liquors on chromatography over Al203 gave 14-chloro-6-
methoxy-Δ6.7-dihydrodeoxycodeine, m. 164-5°, [α]D -235°, thebaine, and IV, m.
173-4°, [a]D -307°. However, 6 q. II in a Vilsmeier reaction at 40° and
hydrolyzed at pH 9 gave 3.7 g. 14-formyloxy-6-methoxy-Δ6.7-
dihydrodeoxycodeine, m. 178-80° (decomposition). Similarly were prepared 6-
ethoxy-7-formyl-14-hydroxy-\Delta 6.7-dihydrodeoxycodeine, m. 220-1°, [\alpha]D -387°,
6-butoxy-7-formyl-15-hydroxy-Δ6.7-dihydrodeoxycodeine, m. 144-4.5°, [α]D -317-
7-formyl-14-hydroxy-6-morpholino-Δ6.7-dihydrodeoxycodeine, m. 174-5°, [α]D -
286°, and
7-formyl-14-hydroxy-6-pyrrolidino-\( \Delta 6.7-\) dihydrodeoxycodeine, m. 241-3°, \( \alpha \) D -
567°. Reduction of 7-formyl compds. gave the corresponding primary alcs.
which were acetylated. Thus 20 g. V in 100 ml. tetrahydrofuran was reduced
with 3 g. LiBH4 to give 85% 14-hydroxy-7-hydroxymethyl-Δ6.7-
dihydrodeoxycodeine (VI), m. 164-5, [a]D -251°. Similarly were prepared 6-
ethoxy-14-hydroxy-7-hydroxymethyl-A6.7-dihydrodeoxycodeine, m. 122-3°, [\alpha]D -
6-chloro-14-hydroxy-7-hydroxymethyl-\Delta6.7-dihydrodeoxycodeine, m. 208-9°, and
6-dimethylamino-
14-hydroxy-7-hydroxymethyl-A6.7-dihydrodeoxycodeine borane adduct, m. 300°
(decomposition). Acetylation of 0.5 g. VI with 0.16 ml. Ac20 and 3 ml.
pyridine at room temperature 16 hrs. gave 0.32 g. 7-acetoxymethyl-14-hydroxy-
6-methoxy-\Delta6.7-dihydrodeoxycodeine, m. 154.5-56°. Other esters of VI prepared
were: 7-diethylacetate, m. 91-2°, 7-o-toluate, m. 123-4°, 7-
phenyldiethylacetate, m. 128-9°, and 7-propionate, m. 108-9°. Similarly were
prepared 7-benzovloxv-6-ethoxv-14-hydroxv-\Delta6.7-dihydrodeoxycodeine, m. 128-
8.5°, and 7-furoate, m. 100-1°. Acid hydrolysis of 7-formyl-6-enol ethers was
carried out by dissolving 0.15 g. compound in 0.5 ml. concentrated HCl.
keeping the mixture at room temperature 15 min., and basifying to pH 9.5 to
give amorphous 14-hydroxy-7-hydroxymethylenedihydrocodeinone (VII) which as
expected was soluble in alkali and gave a purple color with FeCl3 and a
typical spectrum of an enolic \beta-dicarbonyl compound VII was also obtained by
dissolving 0.5 g. 7-formyl-6-enol ether in 1 ml. NaOH, keeping at room
temperature for a few min., and acidifying to pH 9.5. A solution of I g. VII
in 50 ml. H2O containing slightly more than i equivalent NaOH was stirred with
2 ml. MeI for 48 hrs. at room temperature to give 0.4 g. 14-hydroxy-7-
methyldihydrocodeinone, m. 226-8° (decomposition), [\alpha]D -187°, which was also
obtained by methylation of I with MeI-NaNH2 in liquid NH3 solution Hydrolysis
of 6-dialkylamino-7-formyl-14-hydroxydihydrodeoxycodeine derivs. was carried
out by dissolving 0.5 g. compds. in excess 5N HCl, keeping at room
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temperature, basifying to pH 9.5, and chromatographing the product on AlcOa to

give the starting material, 6-dialkylamino-14 -hydroxy-Δ6.7dihydrodeoxycodeine and I, m. 218-19. More vigorous treatment with HCl gave only I. When treated with slight excess of EtOH-NaOH for 30 min. the only product was VII. The formyl compds. (V) gave 96% yield of the oxime, 14hydroxy-7-hydroxyiminomethyl-6- methoxydihydrodeoxycodeine, m. 242-3°, [α]D -216°. Heating 4 g. of the oxime with 25 ml. Ac20 1 hr. gave 2.9 g. 14-acetoxy-7cyano-6-methoxy- $\Delta$ 6.7-dihydrodeoxycodeine, m. 176-6.5°, [ $\alpha$ ]D -305°, which on hydrolysis with 1 equivalent EtOH-NaOH gave 7-cyano-14-hydroxy-6-methoxy-\( \Delta \)6.7dihydrodeoxycodeine, m. 233-5°,  $[\alpha]D$  -311°. On heating 1 g. oxime with 4 ml. concentrated HCl at 60° for 20 min, was obtained isoxazoly1-[6,7-d]-14hydroxydihydrodeoxycodeine, m. 189-90°, [a]D -336°. The structure was proposed on the basis of its insolubility in NaOH and its infrared spectrum. The compound V gave 82% yield of semicarbazone, m. 268-70° (decomposition), which (0.5 g.) on heating with dilute HCl at 100° for 2 hrs. gave 0.3 g. pyrazolinyl[6,7-c]-14-hydroxydihydrodeoxycodeine, m. 290° (decomposition). It was also obtained by refluxing 1 g. V and 0.3 g. NH2NH2.HCl in 50 ml. EtOH 2 hrs, and basifying the solution with Na2CO3. The OMe group in V was easily replaced by heating it with ureas. Thus a solution of 1 g. V and 0.33 g. butylurea in 50 ml. EtOH containing 2 ml. HOAc was refluxed 2 hrs. to give 0.9 q. butylureido-7-formyl-14- hydroxy-Δ6.7-dihydrodeoxycodeine, m. 250-2° (decomposition), [a]D -486°. Similarly were prepared 6-tert-butylureido-7formyl14-hydroxy-Δ6.7-dihydrodeoxycodeine, m. 268°, and 6-(N,Ndiethylinreido)-7-formyl-14-hydroxy-Δ6.7- dihydrodeoxycodeine, m. 220°. Since II did not react under these conditions the activating effect of the 7-formyl group was apparent. Reaction of V with PhNH2 yielded 3 distinct products depending on the conditions used. A solution of 1 g. V and 0.26 ml. (equimolar quantity) PhNH2 in a min, volume MeOH was refluxed 30 min, to give 0.78 g. of the normal anil, 14-hydroxy-6-methoxy-7-phenyliminomethyl- $\Delta 6.7$ dihydrodeoxycodeine, m. 176-7°. Longer reaction with excess PhNH2 led to replacement of the OMe by the anilino group. Thus a solution of 0.5 g. anil and 0.13 ml. PhNH2 in MeOH was refluxed 16 hrs. to give 0.32 g. 6-anilino-7formyl-14-hydroxy-A6.7-dihydrodeoxycodeine, m. 280° (decomposition). It was also formed by heating 1 q. V with 1 q. aniline sulfate in 100 ml. EtOH 4 hrs. In the presence of acid a quinoline was obtained. Thus, a solution of 0.5 g. anil, 0.13 g. PhNH2, and a trace of aniline hydrochloride in EtOH was refluxed 16 hrs. to give 0.88 g. quinolino [6,7-b]-14-hydroxydihydrodeoxycodeine, m. 280° (decomposition). The anil and p-C1C2H4NH2 similarly gave 6'chloroquinolino [6,7b]-14-hydroxydihydrodeoxycodeine, m. 285° (decomposition). The anil was recovered by boiling several hrs. in EtOH. The mechanism of formation of quinoline derivs. was discussed in detail. The Vilsmeier reaction of I was next studied. A solution of 12 g. I in 1,2-dichloroethane was added to a solution of 12 ml. POC13 and 20 ml. HCONMe2 in the same solvent, the mixture heated at 70° 7 hrs., and product hydrolyzed to give 2.4 q. IV, 1.8 q. 6-dimethylamino-7-formyl-14-hydroxy-Δ6.7-dihydrodeoxycodeine (VIII), m. 258° (decomposition),  $[\alpha]D$  -2°, and 1.2 g. of a dimeric product (IX), m. 192-3° (decomposition), [a]D -290°. The yields of IV and IX were the same whether hydrolysis was carried out at pH 4-6 or pH 10, but VIII was not isolated when acid hydrolysis was carried out. The yield of IX increased at the expense of IV and VIII if I was added to the reaction mixture immediately before hydrolysis. IV could not be converted into VIII nor could the vield of VIII be improved by adding Me2NH before hydrolysis. The mechanism of reaction of all these reactions was discussed. The structure of IX was demonstrated by its cleavage in acid solution or on fusion to vield equimolar mixture of IV and I, and finally by its synthesis by the action of IV and I in MeOH containing NaOMe at room temperature. The ultraviolet and infrared spectra of most of the compds. were given and discussed in detail.

OREF 61:5705h,5706a-h,5707a-f

- ${\tt TI} {\tt Vilsmeier}$  reactions with 14-hydroxydihydrocodeinone and derived enol ethers
- AU Lester, M. G.; Petrow, V.; Stephenson, O. CS Brit. Drug Houses Ltd., London
- SO Tetrahedron (1964), 20(6), 1407-17 CODEN: TETRAB; ISSN: 0040-4020

DT Journal

LA Unavailable

OS CASREACT 61:32654

IT 7096-91-5P, 5,10c-(Iminoethano)-10cH-

furo[2',3',4',5':4,5]phenanthro[3,2-c]pyrazol-5aβ(6H)-ol, 4,5α,9,9bβ-tetrahydro-1-methoxy-13-methy1-

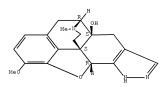
RL: PREP (Preparation)

(preparation of)

RN 7096-91-5 CAPLUS

CN 5,10c-(Iminoethano)-10cH-furo[2',3',4',5':4,5]phenanthro[3,2-c]pyrazol-5a(6H)-ol, 4,5,9,9b-tetrahydro-1-methoxy-13-methyl-, (5R,5aS,9bR,10cS)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.



# OSC.G 2 THERE ARE 2 CAPLUS RECORDS THAT CITE THIS RECORD (2 CITINGS)

=> d abs fbib hitstr 5-9

- L7 ANSWER 5 OF 15 CAPLUS COPYRIGHT 2010 ACS on STN
- AB Addn. of the 4-fluorophenylpyrazole group to the previously described 2azadecalin glucocorticoid receptor (GR) antagonist l resulted in significantly enhanced functional activity. SAR of the bridgehead substituent indicated that whereas groups as small as Me afforded high GR binding, GR functional activity was enhanced by larger groups such as benzyl, substituted ethers, and aminoalkyl derivs. GR antagonists with binding and functional activity comparable to mifepristone were discovered (e.g., 52: GR binding Ki 0.7 nM; GR reporter gene functional Ki 0.6 nM) and found to be highly selective over other steroid receptors. Analogs 43 and 45 had >50% oral bioavailability in the dog.
- AN 2008:232071 CAPLUS Full-text
- DN 148:440269
- TI 1H-Pyrazolo[3,4-g]hexahydro-isoquinolines as selective glucocorticoid receptor antagonists with high functional activity
- AU Clark, Robin D.; Ray, Nicholas C.; Williams, Karen; Blaney, Paul; Ward, Stuart; Crackett, Peter H.; Hurley, Christopher; Dyke, Hazel J.; Clark, David E.; Lockey, Peter; Devos, Rene; Wong, Melanie; Porres, Soraya S.; Bright, Colin P.; Jenkins, Robert E.; Belanoff, Joseph

- CS Corcept Therapeutics, Menlo Park, CA, 94025, USA
- SO Bioorganic & Medicinal Chemistry Letters (2008), 18(4), 1312-1317 CODEN: BMCLE8; ISSN: 0960-894X
- PB Elsevier Ltd.
- DT Journal
- LA English
- OS CASREACT 148:440269
- IT 864972-02-1P 864972-29-2P 864972-39-4P

864972-43-0P 864972-55-4P 1018679-76-9P

RL: DMA (Drug mechanism of action); PAC (Pharmacological activity); PKT (Pharmacokinetics); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(1H-pyrazolo[3,4-g]hexahydro-isoquinolines as selective glucocorticoid receptor antagonists)

RN 864972-02-1 CAPLUS

Absolute stereochemistry.

- RN 864972-29-2 CAPLUS
- CN 1H-Pyracolo[3,4-g]isoquinoline, 6-[[4-(1,1-dimethylethyl)phenyl]sulfonyl]-1-(4-fluorophenyl)-4,4a,5,6,7,8-hexahydro-4a-(methoxymethyl)-, (4aR)- (CA INDEX NAME)

Absolute stereochemistry.

- RN 864972-39-4 CAPLUS
- CN IR-Pyrazolo[3, 4-g]isoquinoline, 1-(4-fluorophenyl)-6-[(4-fluorophenyl)sulfonyl]-4, 4a, 5, 6, 7, 8-hexahydro-4a-(methoxymethyl)-, (4aR)-(CA INDEX NAME)

- RN 864972-43-0 CAPLUS
- CN 1H-Pyrazolo[3,4-g]isoquinoline, 1-(4-fluorophenyl)-4,4a,5,6,7,8-hexahydro-4a-(methoxymethyl)-6-(phenylsulfonyl)-, (4aR)- (CA INDEX NAME)

- RN 864972-55-4 CAPLUS
- CN 1H-Pyrazolo[3,4-g]isoquinoline, 6-[[4-(1,1-dimethylethyl)phenyl]sulfonyl]-1-(4-fluorophenyl)-4,4a,5,6,7,8-hexahydro-4a-(4-morpholinylmethyl)-, (4a5)- (CA INDEX NAME)

Absolute stereochemistry.

- RN 1018679-76-9 CAPLUS
- CN 1H-Pyrazolo[3,4-g]isoquinoline, 1-(4-fluorophenyl)-4,4a,5,6,7,8-hexahydro-4a-(methoxymethyl)-6-[[4-(trifluoromethyl)phenyl]sulfonyl]-, (4aR)- (CA INDEX NAME)

IT 864971-93-7P 864972-25-8P 864972-26-9P 864972-28-1P

RL: DMA (Drug mechanism of action); PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(IH-pyrazolo[3,4-g]hexahydro-isoquinolines as selective glucocorticoid receptor antagonists)

RN 864971-93-7 CAPLUS

CN 1H-Pyrazolo[3,4-g]isoquinoline, 1-(4-fluorophenyl)-4a-[(4-fluorophenyl)methyl]-4,4a,5,6,7,8-hexahydro-6-(phenylmethyl)- (CA INDEX NAME)

- RN 864972-25-8 CAPLUS
- CN 4aH-Pyrazolo[3,4-g]isoquinoline-4a-methanol,
  6-[[4-(1,1-dimethyl=thyl)phenyl]sulfonyl]-1-(4-fluorophenyl)-1,4,5,6,7,8hexahydro-, (4aR)- (CA INDEX NAME)

- RN 864972-26-9 CAPLUS
- CN 4aH-Pyrazolo[3,4-g]isoquinoline-4a-methanol,
  1-(4-fluorophenyl)-6-[(4-fluorophenyl)sulfonyl]-1,4,5,6,7,8-hexahydro-,
  (4aR)- (CA INDEX NAME)

RN 864972-28-1 CAPLUS

CN 4aH-Pyrazolo[3,4-g]isoquinoline-4a-methanol, 1-(4-fluorophenyl)-1,4,5,6,7,8-hexahydro-6-(phenylsulfonyl)-, (4aR)- (CA INDEX NAME)

Absolute stereochemistry.

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IT
     864971-84-6P
                  864972-04-3P
                                  864972-05-4P
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     RL: DMA (Drug mechanism of action); PAC (Pharmacological activity); SPN
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(Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses) (1H-pyrazolo[3,4-g]hexahydro-isoquinolines as selective glucocorticoid

(IH-pyrazolo[3,4-g]hexahydro-isoquinolines as selective glucocorticoic receptor antagonists)

RN 864971-84-6 CAPLUS

RN 864972-04-3 CAPLUS

CN 1H-Pyrazolo[3,4-g]isoquinoline, 1-(4-fluorophenyl)-4,4a,5,6,7,8-hexahydro-4a-methyl-6-[(4-methylphenyl)sulfonyl]-, (4aS)- (CA INDEX NAME)

Absolute stereochemistry.

RN 864972-05-4 CAPLUS

CN 1H-Pyrazolo[3,4-g]isoquinoline, 1-(4-fluorophenyl)-4,4a,5,6,7,8-hexahydro-4a-methyl-6-[[4-(trifluoromethyl)phenyl]sulfonyl]-, (4aS)- (CA INDEX NAME)

Absolute stereochemistry.

RN 864972-09-8 CAPLUS

CN 1H-Pyrazolo[3,4-g]isoquinoline, 1-(4-fluorophenyl)-4,4a,5,6,7,8-hexahydro-6-[(4-methoxyphenyl)sulfonyl]-4a-methyl-, (4aS)- (CA INDEX NAME)

RN 864972-10-1 CAPLUS

CN 1H-Pyrazolo[3,4-g]isoquinoline, 1-(4-fluorophenyl)-6-[(4-fluorophenyl)sulfonyl]-4,4a,5,6,7,8-hexahydro-4a-methyl-, (4aS)- (CA INDEX NAME)

Absolute stereochemistry.

RN 864972-11-2 CAPLUS

CN 1H-Pyrazolo[3,4-g]isoquinoline, 1-(4-fluorophenyl)-6-[(2-fluorophenyl)sulfonyl]-4,4a,5,6,7,8-hexahydro-4a-methyl-, (4aS)- (CA INDEX NAME)

Absolute stereochemistry.

- RN 864972-12-3 CAPLUS
- CN 1H-Pyrazolo[3,4-g]isoquinoline, 1-(4-fluorophenyl)-4,4a,5,6,7,8-hexahydro-4a-methyl-6-[(2-methylphenyl)sulfonyl]-, (4aS)- (CA INDEX NAME)

Absolute stereochemistry.

- RN 864972-19-0 CAPLUS
- CN Benzenamine, 4-[((4aS)-1-(4-fluoropheny1)-1,4,4a,5,7,8-hexahydro-4a-methyl-6H-pyrazolo[3,4-g]isoquinolin-6-yl]sulfonyl]- (CA INDEX NAME)

RN 864972-30-5 CAPLUS

CN 1H-Pyrazolo[3,4-g]isoquinoline, 6-[[4-(1,1-dimethylethyl)phenyl]sulfonyl]-1-(4-fluorophenyl)-4,4a,5,6,7,8-hexahydro-4a-[(2-methoxyethoxy)methyl]-, (4aR)- (CA INDEX NAME)

Absolute stereochemistry.

RN 864972-32-7 CAPLUS

CN 1H-Pyracolo[3,4-g]isoquinoline, 6-[[4-(1,1-dimethylethyl)phenyl]sulfonyl]-4a-(ethoxymethyl)-1-(4-fluorophenyl)-4,4a,5,6,7,8-hexahydro-, (4aR)- (CA INDEX NAME)

Absolute stereochemistry.

RN 864972-33-8 CAPLUS

CN 1H-Pyrazolo[3,4-g]isoquinoline, 6-[[4-(1,1-dimethylethyl)phenyl]sulfonyl]-1-(4-fluorophenyl)-4,4a,5,6,7,8-hexahydro-4a-[(3-methoxypropoxy)methyl]-, (4aR)- (CA INDEX NAME)

- RN 864972-34-9 CAPLUS
- CN Propanenitrile, 3-[[(4aR)-6-[[4-(1,1-dimethylethyl)phenyl]sulfonyl]-1-(4-fluorophenyl)-1,4,5,6,7,8-hexahydro-4aH-pyrazolo[3,4-g]isoquinolin-4a-yl]methoxy]- (CA INDEX NAME)

- RN 864972-36-1 CAPLUS
- CN 1R-Pyrazolo[3, 4-g]isoquinoline, 6-[[4-(1,1-dimethylethyl)phenyl]sulfonyl]-1-(4-fluorophenyl)-4, 4a, 5, 6, 7, 8-hexahydro-4a-[[2-(1piperidinyl)ethoxy|methyl]-, (4aR)- (CA INDEX NAME)

Absolute stereochemistry.

- RN 864972-37-2 CAPLUS
- CN 1H-Pyrazolo[3,4-g]isoguinoline, 6-[[4-(1,1-dimethylethyl)phenyl]sulfonyl]-1-(4-fluorophenyl)-4,4a,5,6,7,8-hexahydro-4a-[[2-(1pyrrolidinyl)ethoxy]methyl]-, (4aR)- (CA INDEX NAME)

RN 864972-38-3 CAPLUS

CN 1H-Pyrazolo[3,4-g]isoquinoline, 1-(4-fluoropheny1)-6-[(4-fluoropheny1)sulfony1]-4,4a,5,6,7,8-hexahydro-4a-[(2-methoxyethoxy)methy1]-, (4aR)- (CA INDEX NAME)

Absolute stereochemistry.

RN 864972-40-7 CAPLUS

CN 1H-Pyrazolo[3,4-g]isoquinoline, 1-(4-fluorophenyl)-4,4a,5,6,7,8-hexahydro-4a-(methoxymethyl)-6-[(4-methylphenyl)sulfonyl]-, (4aR)- (CA INDEX NAME)

Absolute stereochemistry.

RN 864972-41-8 CAPLUS

CN 1H-Pyrazolo[3,4-g]isoquinoline, 1-(4-fluorophenyl)-4,4a,5,6,7,8-hexahydro-4a-[(2-methoxyethoxy)methyl]-6-[(4-methylphenyl)sulfonyl]-, (4aR)- (CA INDEX NAME)

- RN 864972-42-9 CAPLUS
- CN 1H-Pyrazolo[3,4-g]isoquinoline, 1-(4-fluorophenyl)-4,4a,5,6,7,8-hexahydro-4a-[(2-methoxyethoxy)methyl]-6-(phenylsulfonyl)-, (4aR)- (CA INDEX NAME)

- RN 864972-54-3 CAPLUS
- CN 4aH-Pyrazolo[3,4-g]isoquinoline-4a-methanamine, 6-[[4-(1,1-dimethyl=thyl]phenyl]sulfonyl]-1-(4-fluorophenyl)-1,4,5,6,7,8hexahydro-N,N-dimethyl-, (4a8)- (CA INDEX NAME)

Absolute stereochemistry.

- RN 864972-58-7 CAPLUS
- CN 1H-Pyrazolo[3,4-g]isoquinoline, 6-[[4-(1,1-dimethylethyl)phenyl]sulfonyl]-1-(4-fluorophenyl)-4,4a,5,6,7,8-hexahydro-4a-(1-pyrrolidinylmethyl)-, (4aS)- (CA INDEX NAME)

RN 864972-59-8 CAPLUS

CN 4aH-Pyrazolo[3,4-g]isoquinoline-4a-methanamine,
6-[(4-(1,1-dimethylethyl)phryl]sulfonyl]-N-ethyl-1-(4-fluorophenyl)1,4,5,6,7,8-hexhydro-, (4aS)- (CA INDEX NAME)

Absolute stereochemistry.

RN 864972-60-1 CAPLUS

CN 4AH-Pyrazolo[3,4-g]isoquinoline-4a-methanamine,
6-[[4-(1,1-dimethylethyl)phenyl]sulfonyl]-N,N-diethyl-1-(4-fluorophenyl)1,4,5,6,7,8-hexahydro-, (4aS)- (CA INDEX NAME)

Absolute stereochemistry.

RN 864972-61-2 CAPLUS

CN 1H-Pyrazolo[3, 4-g]isoquinoline, 6-[[4-(1,1-dimethylethyl)phenyl]sulfonyl]-1-(4-fluorophenyl)-4, 4a, 5, 6, 7, 8-hexahydro-4a-(1-piperidinylmethyl)-, (4aS)- (CA INDEX NAME)

- RN 864972-62-3 CAPLUS
- CN 4aH-Pyrazolo[3,4-g]isoquinoline-4a-methanamine,
  6 [[4-(1,1-dimethyl=thyl]phenyl]sulfonyl]-1-(4-fluorophenyl)-1,4,5,6,7,8hexahydro-N-(2-methoxyethyl)-, (4a5)- (CA INDEX NAME)

- RN 864972-63-4 CAPLUS
- CN 1H-Pyrazolo[3, 4-g]isoquinoline, 6-[[4-(1,1-dimethylethyl)phenyl]sulfonyl]-1-(4-fluorophenyl)-4, 4a, 5, 6, 7, 8-hexahydro-4a-[(4-methyl-1piperazinyl)methyl]-, (4a8)- (CA INDEX NAME)

Absolute stereochemistry.

- RN 864972-64-5 CAPLUS
- CN 1,2-Ethanediamine, N2-[[(4aS)-6-[[4-(1,1-dimethylethyl)phenyl]sulfonyl]-1-(4-fluorophenyl)-1,4,5,6,7,8-hexahydro-4aH-pyrazolo[3,4-g]isoquinolin-4ayl]methyl]-N1,N1-dimethyl- (CA INDEX NAME)

- RN 864972-69-0 CAPLUS
- CN 4AH-Pyrazolo[3,4-g]isoquinoline-4a-methanamine,
  6-[[4-(1,1-dimethylethyl)phenyl]sulfonyl]-1-(4-fluorophenyl)-1,4,5,6,7,8hexahydro-N-(1-methylethyl)-, (4a5)- (CA INDEX NAME)

- RN 864972-70-3 CAPLUS
- CN 1H-Pyrazolo[3,4-g]isoquinoline, 4a-(1-azetidinylmethyl)-6-[[4-(1,1-dimethylethyl)phenyl]sulfonyl]-1-(4-fluorophenyl)-4,4a,5,6,7,8-hexahydro-,(4a5)- (CA INDEX NAME)

Absolute stereochemistry.

- RN 864972-71-4 CAPLUS
- CN 4aH-Pyrazolo[3,4-g]isoquinoline-4a-methanamine,
  6-[[4-(1,1-dimethylethyl)phenyl]sulfonyl]-1-(4-fluorophenyl)-1,4,5,6,7,8hexahydro-N-2-propen-1-yl-, (4aS)- (CA INDEX NAME)

RN 864972-72-5 CAPLUS

CN Ethanol, 2-[[(4aS)-6-[[4-(1,1-dimethylethyl)phenyl]sulfonyl]-1-(4-fluorophenyl)-1,4,5,6,7,8-hexahydro-4aH-pyrazolo[3,4-g]isoquinolin-4a-yl]methyl]amino]- (CA INDEX NAME)

Absolute stereochemistry.

RN 864972-75-8 CAPLUS

CN 4aH-Pyrazolo[3,4-g]isoquinoline-4a-methanamine, 1-(4-fluorophenyl)-6-[(4-fluorophenyl)sulfonyl]-1,4,5,6,7,8-hexahydro-N,N-dimethyl-, (4aS)- (CA INDEX NAME)

Absolute stereochemistry.

RN 864972-76-9 CAPLUS

CN 1H-Pyrazolo[3,4-g]isoquinoline, 1-(4-fluorophenyl)-6-[(4-fluorophenyl)sulfonyl]-4,4a,5,6,7,8-hexahydro-4a-(1-pyrrolidinylmethyl)-, (4aS)- (CA INDEX NAME)

RN 864972-77-0 CAPLUS

CN 1H-Pyrazolo[3,4-g]isoquinoline, 1-(4-fluorophenyl)-4,4a,5,6,7,8-hexahydro-6-(phenylsulfonyl)-4a-(1-pyrrolidinylmethyl)-, (4aS)- (CA INDEX NAME)

Absolute stereochemistry.

RN 864972-78-1 CAPLUS

CN 4aH-Pyrazolo[3, 4-g]isoquinoline-4a-methanamine, 1-(4-fluorophenyl)-1,4,5,6,7,8-hexahydro-N,N-dimethyl-6-(phenylsulfonyl)-, (4a5)- (CA INDEX NAME)

Absolute stereochemistry.

RN 864972-79-2 CAPLUS

CN 1H-Pyrazolo[3,4-g]isoquinoline, 1-(4-fluorophenyl)-4,4a,5,6,7,8-hexahydro-4a-(4-morpholinylmethyl)-6-(phenylsulfonyl)-, (4aS)- (CA INDEX NAME)

- RN 864972-85-0 CAPLUS
- CN 1H-Pyrazolo[3,4-g]isoquinoline, 1-(4-fluorophenyl)-4,4a,5,6,7,8-hexahydro-6-(phenylsulfonyl)-4a-(1-piperidinylmethyl)-, (4aS)- (CA INDEX NAME)

- RN 864973-27-3 CAPLUS
- CN 1H-Pyrazolo[3,4-g]isoquinoline, 6-[[4-(1,1-dimethylethyl)phenyl]sulfonyl]-1-(4-fluorophenyl)-4a-[(4-fluorophenyl)methyl]-4,4a,5,6,7,8-hexahydro-(CA INDEX NAME)

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- RN 864973-28-4 CAPLUS
- CN 1H-Pyrazolo[3,4-g]isoquinoline, 1-(4-fluorophenyl)-4a-[(4-fluorophenyl)methyl]-4,4a,5,6,7,8-hexahydro-6-(phenylsulfonyl)- (CA INDEX NAME)

- RN 864973-29-5 CAPLUS
- CN 1H-Pyrazolo[3,4-g]isoquinoline, 1-(4-fluorophenyl)-4a-[(4fluorophenyl)methyl]-4,4a,5,6,7,8-hexahydro-6-[(4-methylphenyl)sulfonyl]-(CA INDEX NAME)

- RN 864973-30-8 CAPLUS
- CN 1H-Pyrazolo[3,4-g]isoquinoline, 1-(4-fluorophenyl)-4a-[(4fluorophenyl)methyl]-6-[(4-fluorophenyl)sulfonyl]-4,4a,5,6,7,8-hexahydro-(CA INDEX NAME)

- RN 864973-31-9 CAPLUS
- CN 1R-Pyrazolo[3,4-g]isoquinoline, 1-(4-fluorophenyl)-4a-[(4-fluorophenyl)methyl]-4,4a,5,6,7,8-hexahydro-6-(methylsulfonyl)- (CA INDEX NAME)

RN 864973-32-0 CAPLUS

CN 1H-Pyrazolo[3,4-g]isoquinoline, 6-(buty1sulfony1)-1-(4-fluoropheny1)-4a[(4-fluoropheny1)methy1]-4,4a,5,6,7,8-hexahydro- (CA INDEX NAME)

RN 864973-36-4 CAPLUS

CN 1H-Pyrazolo[3,4-g]isoquinoline, 6-[[6-(1,1-dimethylethyl)-3-pyridinyl]sulfonyl]-1-(4-fluorophenyl)-4-[(4-fluorophenyl)-4-[4,5,6,7,8-hexahydro-(CA INDEX NAME)

RN 864973-37-5 CAPLUS

CN 1H-Pyrazolo[3,4-g]isoquinoline, 1-(4-fluorophenyl)-4a-[(4-fluorophenyl)methyl]-4,4a,5,6,7,8-hexahydro-6-[[4-(4-morpholinyl)phenyl]sulfonyl]- (CA INDEX NAME)

RN 864973-38-6 CAPLUS

CN 1H-Pyrazolo[3,4-g]isoquinoline, 1-(4-fluorophenyl)-4a-[(4-fluorophenyl)methyl]-4,4a,5,6,7,8-hexahydro-6-(4-pyridinylmethyl)- (CA INDEX NAME)

RN 864973-39-7 CAPLUS

CN 1H-Pyrazolo[3,4-g]isoquinoline, 1-(4-fluorophenyl)-4a-[(4-fluorophenyl)methyl]-4,4a,5,6,7,8-hexahydro-6-(3-pyridinylmethyl)- (CA INDEX NAME)

RN 864973-40-0 CAPLUS

CN 1H-Pyrazolo[3,4-g]isoquinoline, 1-(4-fluorophenyl)-4a-[(4-fluorophenyl)methyl]-4,4a,5,6,7,8-hexahydro-6-(2-pyridinylmethyl)- (CA INDEX NAME)

RN 864973-45-5 CAPLUS

CN 1H-Pyrazolo[3,4-g]isoquinoline, 1-(4-fluorophenyl)-4a-[(4-fluorophenyl)methyl]-4,4a,5,6,7,8-hexahydro-6-phenyl- (CA INDEX NAME)

RN 864973-47-7 CAPLUS

CN 6H-Pyrazolo[3,4-g]isoquinoline-6-sulfonamide, 1-(4-fluorophenyl)-4a-[(4-fluorophenyl)methyl]-1,4,4a,5,7,8-hexahydro-N-phenyl- (CA INDEX NAME)

RN 864973-48-8 CAPLUS

CN 1H-Pyrazolo[3,4-g]isoquinoline, 1-(4-fluorophenyl)-4a-[(4-fluorophenyl)methyl]-4,4a,5,6,7,8-hexahydro-6-(4-morpholinylsulfonyl)-(CA INDEX NAME)

- RN 1018679-69-0 CAPLUS
- CN Methanone, [1-(4-fluorophenyl)-4a-[(4-fluorophenyl)methyl]-1,4,4a,5,7,8hexahydro-6H-pyrazolo[3,4-g]isoquinolin-6-yl]phenyl- (CA INDEX NAME)

- RN 1018679-79-2 CAPLUS
- CN 1H-Pyrazolo[3,4-g]isoquinoline, 4a-(ethoxymethyl)-1-(4-fluorophenyl)-4,4a,5,6,7,8-hexahydro-6-[[4-(trifluoromethyl)phenyl]sulfonyl]-, (4aR)-(CA INDEX NAME)

- RN 1018679-81-6 CAPLUS
- CN 1H-Pyrazolo[3,4-g]isoquinoline, 1-(4-fluorophenyl)-4,4a,5,6,7,8-hexahydro-4a-(propoxymethyl)-6-[[4-(trifluoromethyl)phenyl]sulfonyl]-, (4aR)- (CA INDEX NAME)

RN 1018679-85-0 CAPLUS

CN Ethanol, 2-[(4aR)-6-[(4-(1,1-dimethylethyl)phenyl]sulfonyl]-1-(4-fluorophenyl)-1,4,5,6,7,8-hexahydro-4aH-pyrazolo[3,4-g]isoquinolin-4a-yl]methoxyl- (CA INDEX NAME)

Absolute stereochemistry.

IT 864972-01-0P 864972-21-4P 364972-53-2P

1018679-86-1P 1018679-87-2P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(1H-pyrazolo[3,4-g]hexahydro-isoquinolines as selective glucocorticoid receptor antagonists)

RN 864972-01-0 CAPLUS

CN 6H-Pyrazolo[3,4-g]isoquinoline-6-carboxylic acid, 1-(4-fluorophenyl)-1,4,4a,5,7,8-hexahydro-4a-methyl-, 1,1-dimethylethyl ester, (4aS)- (CA INDEX NAME)

Absolute stereochemistry.

RN 864972-21-4 CAPLUS

CN 1H-Pyrazolo(3,4-g)isoquinoline-4a,6(4H,5H)-dicarboxylic acid, 1-(4-fluorophenyl)-7,8-dihydro-, 6-(1,1-dimethylethyl) 4a-methyl ester, (4aR)- (CA INDEX NAME)

RN 864972-53-2 CAPLUS

CN 4aH-Pyrazolo[3,4-g]isoquinoline-4a-carboxaldehyde,
6-[[4-(1,1-dimethyl=thyl)phenyl]sulfonyl]-1-(4-fluorophenyl)-1,4,5,6,7,8hexahydro-, (4aR)- (CA INDEX NAME)

Absolute stereochemistry.

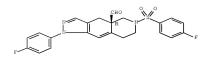
RN 1018679-86-1 CAPLUS

CN 4aH-Pyrazolo[3,4-g]isoquinoline-4a-carboxaldehyde, 1-(4-fluorophenyl)-1,4,5,6,7,8-hexahydro-6-(phenylsulfonyl)-, (4aR)- (CA INDEX NAME)

Absolute stereochemistry.

RN 1018679-87-2 CAPLUS

CN 4aH-Pyrazolo[3,4-g]isoquinoline-4a-carboxaldehyde, 1-(4-fluorophenyl)-6-[(4-fluorophenyl)sulfonyl]-1,4,5,6,7,8-hexahydro-, (4aR)- (CA INDEX NAME)



osc.G THERE ARE 3 CAPLUS RECORDS THAT CITE THIS RECORD (3 CITINGS) RE.CNT 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

ANSWER 6 OF 15 CAPLUS COPYRIGHT 2010 ACS on STN L7

AR Title compds. I [L1 and L2 independently = a bond, O, S, etc.; A = (un) substituted 5-6 membered heterocycloalkyl or heteroaryl; R1 = H, (un) substituted alkyl, heteroalkyl, etc.; R2 = (un) substituted alkyl, heteroalkyl, cycloalkyl, etc.] and their pharmaceutically acceptable salts, are prepared and disclosed as modulators of glucocorticoid receptor. Thus, II was prepared by cyclization of (S)-8a-benzyl-2-(4-tert-butyl-benzenesulfonyl)-7-[1-hydroxy-meth-(Z)- ylidene]-1,3,4,7,8,8a-hexahydro-2H-isoquinolin-6-one (preparation given) with hydrazine hydrate. The activity of I was evaluated in glucocorticoid receptor binding assay and it was revealed that selected compds. of the invention displayed IC50 values in the range of 10 up to 100 nm and others below 10 nM. Pharmaceutical compns. comprising I are disclosed. AN 2005:1021750 CAPLUS Full-text

DN 143:306309

TΙ Preparation of triazacyclopenta[b]naphthalene derivatives as modulators of glucocorticoid receptor

IN Clark, Robin D.; Ray, Nicholas C.; Blaney, Paul M.; Hurley, Christopher A.; Williams, Karen

PA Corcept Therapeutics, Inc., USA

SO PCT Int. Appl., 160 pp.

CODEN: PIXXD2

Patent

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			US 2004-551836P	P 20040309
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ASSIGNMENT HISTORY FOR US PATENT AVAILABLE IN LSUS DISPLAY FORMAT

OS CASREACT 143:306309; MARPAT 143:306309

IT 864972-21-4P 964972-22-5F 964972-53-2P 864972-96-3P 864972-98-5P 864973-03-5P 864973-18-2P 864973-19-3P 864973-20-6P

864973-21-7P 864973-22-8P

RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(preparation of triazacyclopenta[b]naphthalene derivs. as modulators of glucocorticoid receptor)

RN 864972-21-4 CAPLUS

CN lH-Pyrazolo[3,4-g]isoquinoline-4a,6(4H,5H)-dicarboxylic acid, 1-(4-fluorophenyl)-7,8-dihydro-,6-(1,1-dimethylethyl) 4a-methyl ester, (4aR)- (CA INDEX NAME)

Absolute stereochemistry.

- RN 864972-22-5 CAPLUS
- CN 4aH-Pyrazolo[3,4-g]isoquinoline-4a-carboxylic acid, 6-[[4-(1,1-dimethylethyl)phenyl]sulfonyl]-1-(4-fluorophenyl)-1,4,5,6,7,8-hexahydro-, methyl ester, (4aR)- (CA INDEX NAME)

Absolute stereochemistry.

- RN 864972-53-2 CAPLUS
- CN 48H-Pyrazolo[3,4-g]isoquinoline-4a-carboxaldehyde,
  6-[[4-(1,1-dimethylethyl)phenyl]sulfonyl]-1-(4-fluorophenyl)-1,4,5,6,7,8hexahydro-, (4aR)- (CA INDEX NAME)

Absolute stereochemistry.

RN

CN 1H-Pyrazolo[3,4-g]isoquinoline-4a,6(4H,5H)-dicarboxylic acid, 1-(4-fluorophenyl)-7,8,8a,9-tetrahydro-, 6-(1,1-dimethylethyl) 4a-methyl ester, (4aR,8aS)- (CA INDEX NAME)

Absolute stereochemistry.

- RN 864972-98-5 CAPLUS
- CN 4aH-Pyrazolo[3,4-g]isoquinoline-4a-methanol, 6-[[4-(1,1-dimethylethyl)phenyl]sulfonyl]-1-(4-fluorophenyl)-1,4,5,6,7,8,8a,9-octahydro-, (4aR,8aS)- (CA INDEX NAME)

Absolute stereochemistry.

- RN 864973-03-5 CAPLUS
- CN 48H-Pyrazolo[3,4-g]isoquinoline-4a-carboxylic acid,
  6-[[4-(1,1-dimethylethyl)phenyl]sulfonyl]-1-(4-fluorophenyl)-1,4,5,6,7,8hexahydro-, (4aR)- (CA INDEX NAME)

Absolute stereochemistry.

- RN 864973-18-2 CAPLUS
- CN 1H-Pyrazolo[3,4-g]isoquinoline, 6-[[4-(1,1-dimethylethyl)phenyl]sulfonyl]-4a-(1,3-dithian-2-ylidenemethyl)-1-(4-fluorophenyl)-4,4a,5,6,7,8-hexahydro-,(4aR)- (CA INDEX NAME)

$$\begin{array}{c|c} & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & \\ & & & \\ & &$$

- RN 864973-19-3 CAPLUS
- CN 4aH-Pyrazolo[3,4-g]isoquinoline-4a-acetic acid,
  6-[[4-(1,1-dimethyl=thyl]phenyl]sulfonyl]-1-(4-fluorophenyl)-1,4,5,6,7,8hexahydro-, methyl ester, (4aR)- (CA INDEX NAME)

- RN 864973-20-6 CAPLUS
- CN 4aH-Pyrazolo[3,4-g]isoquinoline-4a-ethanol,
  6-[[4-(1,1-dimethylethyl)phenyl]sulfonyl]-1-(4-fluorophenyl)-1,4,5,6,7,8hexahydro-, (4aR)- (CA INDEX NAME)

Absolute stereochemistry.

- RN 864973-21-7 CAPLUS
- CN 1H-Pyrazolo[3,4-g]isoquinoline, 6-[[4-(1,1-dimethylethyl)phenyl]sulfonyl]-1-(4-fluorophenyl)-4,4a,5,6,7,8-hexahydro-4a-(2-methoxyethyl)-, (4aR)-(CA INDEX NAME)

RN 864973-22-8 CAPLUS

N 4aH-Pyrazolo[3,4-g]isoquinoline-4a-acetaldehyde, 6-[[4-(1,1-dimethylethyl)phenyl]sulfonyl]-1-(4-fluorophenyl)-1,4,5,6,7,8-hexahydro-, (4aR)- (CA INDEX NAME)

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864971-79-9P
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                               864971-81-3P
864971-83-5P
              864971-84-6P
                               864971-85-7P
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864971-92-69
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864973-29-5P
             864973-30-8P
                            364973-31-9P
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                            864973-34-2P
864973-35-3F 864973-36-4P
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864973-44-4P
            864973-45-5P
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864973-47-7P
              864973-48-8P
                           864973-49-9P
864973-50-2P
             864973-51-3P
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RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES

(preparation of triazacyclopenta(b)naphthalene derivs. as modulators of glucocorticoid receptor) RN 864971-79-9 CAPLUS

CN 1H-Pyrazolo[3,4-g]isoquinoline, 6-[[4-(1,1-dimethylethyl)phenyl]sulfonyl]-4,4a,5,6,7,8-hexahydro-4a-(phenylmethyl)- (CA INDEX NAME)

RN 864971-80-2 CAPLUS

CN 1H-Pyrazolo[3,4-g]isoquinoline, 4,4a,5,6,7,8-hexahydro-6-[[4-(4-morpholinyl)phenyl]sulfonyl]-4a-(phenylmethyl)- (CA INDEX NAME)

RN 864971-81-3 CAPLUS

CN 1H-Pyrazolo[3,4-g]isoquinoline, 6-[(3,4-dihydro-4-methyl-2H-1,4-benzoxazin-7-yl)sulfonyl]-4,4a,5,6,7,8-hexahydro-4a-(phenylmethyl)- (CA INDEX NAME)

- RN 864971-83-5 CAPLUS

- RN 864971-84-6 CAPLUS
- CN 1H-Pyrazolo[3,4-g]isoquinoline, 6-[[4-(1,1-dimethylethyl)phenyl]sulfonyl]-1-(4-fluorophenyl)-4,4a,5,6,7,8-hexahydro-4a-(phenylmethyl)-, (4aS)- (CA INDEX NAME)

- RN 864971-85-7 CAPLUS
- CN 1H-Pyrazolo[3,4-g]isoquinoline, 6-[[4-(1,1-dimethylethyl)phenyl]sulfonyl]-4,4a,5,6,7,8-hexahydro-1-(4-methoxyphenyl)-4a-(phenylmethyl)-, (4aS)- (CA INDEX NAME)

- RN 864971-86-8 CAPLUS
- CN 1H-Pyrazolo[3,4-g]isoquinoline, 6-[[4-(1,1-dimethylethyl)phenyl]sulfonyl]-

4,4a,5,6,7,8-hexahydro-1-(4-methylphenyl)-4a-(phenylmethyl)-, (4aS)- (CA INDEX NAME)

- RN 864971-87-9 CAPLUS
- CN 1H-Pyrazolo[3,4-g]isoquinoline, 6-[[4-(1,1-dimethylethyl)phenyl]sulfonyl]4,4a,5,6,7,8-hexahydro-1,4a-bis(phenylmethyl)- (CA INDEX NAME)

$$\begin{array}{c} Ph-CH_2 \\ Ph-CH_2 \\ \end{array}$$

- RN 864971-88-0 CAPLUS
- CN 1H-Pyrazolo[3,4-g]isoquinoline, 6-[[4-(1,1-dimethylethyl)phenyl]sulfonyl]-4,4a,5,6,7,8-hexahydro-4a-(phenylmethyl)-1-[4-(trifluoromethyl)phenyl]-(CA INDEX NAME)

- RN 864971-89-1 CAPLUS
- CN Benzonitrile, 4-[6-[[4-(1,1-dimethylethyl)phenyl]sulfonyl]-4,4a,5,6,7,8-hexahydro-4a-(phenylmethyl)-IH-pyrazolo[3,4-g]isoquinolin-1-yl]- (CA INDEX NAME)

$$\text{NC} = \text{Ph-CH2} \times \text{Ph-CH2}$$

- RN 864971-90-4 CAPLUS
- CN Benzenesulfonamide, 4-[6-[[4-(1,1-dimethylethyl]phenyl]sulfonyl]-4,4a,5,6,7,8-hexahydro-4a-(phenylmethyl)-1H-pyrazolo[3,4-g]isoquinolin-1yl]- (CA INDEX NAME)

- RN 864971-91-5 CAPLUS
- CN 1H-Pyrazolo[3,4-g]isoquinoline, 6-[[4-(1,1-dimethylethyl)phenyl]sulfonyl]-4,4a,5,6,7,8-hexahydro-1-[(3-hydroxyphenyl)methyl]-4a-(phenylmethyl)-(9CI) (CA INDEX NAME)

- RN 864971-92-6 CAPLUS
- CN 1H-Pyrazolo[3,4-g]isoquinoline, 1-(4-fluorophenyl)-4,4a,5,6,7,8-hexahydro-4a,6-bis(phenylmethyl)- (CA INDEX NAME)

- RN 864971-93-7 CAPLUS
- CN 1H-Pyrazolo[3,4-g]isoquinoline, 1-(4-fluorophenyl)-4a-[(4-fluorophenyl)methyl]-4,4a,5,6,7,8-hexahydro-6-(phenylmethyl)- (CA INDEX NAME)

- RN 864971-94-8 CAPLUS
- CN 1H-Pyrazolo[3,4-g]isoquinoline, 1-(4-fluorophenyl)-4,4a,5,6,7,8-hexahydro-4a-[(4-methoxyphenyl)methyl]-6-(phenylmethyl)- (CA INDEX NAME)

- RN 864971-97-1 CAPLUS
- CN 1H-Pyrazolo[3,4-g]isoquinoline, 6-[[4-(1,1-dimethylethyl)phenyl]sulfonyl]-4,4a,5,6,7,8,8a,9-octahydro-4a-(phenylmethyl)-, (4aR,8aR)-rel- (CA INDEX NAME)

Relative stereochemistry.

- RN 864971-98-2 CAPLUS
- CN 1H-Pyrazolo[3,4-g]isoquinoline, 6-[[4-(1,1-dimethylethyl)phenyl]sulfonyl]-1-(4-fluorophenyl)-4,4a,5,6,7,8,8a,9-octahydro-4a-(phenylmethyl)-, (4aR,8aR)-rel- (CA INDEX NAME)

Relative stereochemistry.

- RN 864972-01-0 CAPLUS
- CN 6H-Pyrazolo[3,4-g]isoguinoline-6-carboxylic acid, 1-(4-fluorophenyl)-1,4,4a,5,7,8-hexahydro-4a-methyl-, 1,1-dimethylethyl ester, (4aS)- (CA INDEX NAME)

- RN 864972-02-1 CAPLUS
- CN 1H-Pyrazolo[3,4-g]isoquinoline, 6-[[4-(1,1-dimethylethyl)phenyl]sulfonyl]-1-(4-fluorophenyl)-4,4a,5,6,7,8-hexahydro-4a-methyl-, (4aS)- (CA INDEX NAME)

- RN 864972-03-2 CAPLUS
- CN 1H-Pyrazolo[3,4-g]isoquinoline, 1-(4-fluorophenyl)-4,4a,5,6,7,8-hexahydro-4a-methyl-6-(phenylsulfonyl)-, (4aS)- (CA INDEX NAME)

Absolute stereochemistry.

- RN 864972-04-3 CAPLUS
- CN 1H-Pyrazolo[3,4-g]isoquinoline, 1-(4-fluorophenyl)-4,4a,5,6,7,8-hexahydro-4a-methyl-6-[(4-methylphenyl)sulfonyl]-, (4aS)- (CA INDEX NAME)

RN 864972-05-4 CAPLUS

CN 1H-Pyrazolo[3,4-g]isoquinoline, 1-(4-fluorophenyl)-4,4a,5,6,7,8-hexahydro-4a-methyl-6-[[4-(trifluoromethyl)phenyl]sulfonyl]-, (4aS)- (CA INDEX NAME)

Absolute stereochemistry.

- RN 864972-06-5 CAPLUS
- CN 1H-Pyrazolo[3,4-g]isoquinoline, 1-(4-fluorophenyl)-4,4a,5,6,7,8-hexahydro-4a-methyl-6-[[4-(4-morpholinyl)phenyl]sulfonyl]-, (4aS)- (CA INDEX NAME)

Absolute stereochemistry.

- RN 864972-07-6 CAPLUS
- CN 1H-Pyrazolo[3,4-g]isoquinoline, 6-[(3,4-dihydro-4-methyl-2H-1,4-benzoxazin-7-yl)sulfonyl]-1-(4-floorophenyl)-4,4a,5,6,7,8-hexahydro-4a-methyl-,(4a5)- (CA INDEX NAME)

Absolute stereochemistry.

- RN 864972-08-7 CAPLUS
- CN Benzonitrile, 4-[[(4aS)-1-(4-fluorophenyl)-1,4,4a,5,7,8-hexahydro-4a-methyl-6H-pyrazolo[3,4-g]isoquinolin-6-yl]sulfonyl]- (CA INDEX NAME)

RN 864972-09-8 CAPLUS

CN 1H-Pyrazolo[3,4-g]isoquinoline, 1-(4-fluorophenyl)-4,4a,5,6,7,8-hexahydro-6-[(4-methoxyphenyl)sulfonyl]-4a-methyl-, (4aS)- (CA INDEX NAME)

Absolute stereochemistry.

RN 864972-10-1 CAPLUS

CN 1H-Pyrazolo[3,4-g]isoquinoline, 1-(4-fluoropheny1)-6-[(4-fluoropheny1)sulfony1]-4,4a,5,6,7,8-hexahydro-4a-methy1-, (4aS)- (CA INDEX NAME)

Absolute stereochemistry.

RN 864972-11-2 CAPLUS

CN 1H-Pyrazolo[3,4-g]isoquinoline, 1-(4-fluorophenyl)-6-[(2-fluorophenyl)sulfonyl]-4,4a,5,6,7,8-hexahydro-4a-methyl-, (4aS)- (CA INDEX NAME)

- RN 864972-12-3 CAPLUS
- CN 1H-Pyrazolo[3,4-g]isoquinoline, 1-(4-fluorophenyl)-4,4a,5,6,7,8-hexahydro-4a-methyl-6-[(2-methylphenyl)sulfonyl]-, (4aS)- (CA INDEX NAME)

- RN 864972-13-4 CAPLUS
- CN 1H-Pyrazolo[3,4-g]isoquinoline, 1-(4-fluorophenyl)-4,4a,5,6,7,8-hexahydro-4a-methyl-6-(phenylmethyl)-, (4aS)- (CA INDEX NAME)

Absolute stereochemistry.

- RN 864972-14-5 CAPLUS
- CN 6H-Pyrazolo[3, 4-g]isoquinoline-6-sulfonamide, 1-(4-fluorophenyl)-1, 4, 4a, 5, 7, 8-hexahydro-4a-methyl-N-phenyl-, (4aS)- (CA INDEX NAME)

Absolute stereochemistry.

- RN 864972-15-6 CAPLUS
- CN 1H-Pyrazolo[3,4-g]isoquinoline, 6-[(4,4-dimethyl-1-piperidinyl)sulfonyl]-1-(4-fluorophenyl)-4,4a,5,6,7,8-hexahydro-4a-methyl-, (4aS)- (CA INDEX NAME)

RN 864972-16-7 CAPLUS

CN 1H-Pyrazolo[3,4-g]isoquinoline, 1-(4-fluorophenyl)-4,4a,5,6,7,8-hexahydro-4a-methyl-6-(1-piperidinylsulfonyl)-, (4aS)- (CA INDEX NAME)

Absolute stereochemistry.

RN 864972-17-8 CAPLUS

CN 1H-Pyrazolo[3,4-g]isoquinoline, 6-[[4-(1,1-dimethylethyl)phenyl]sulfonyl]-4,4a,5,6,7,8-hexahydro-4a-methyl-1-(4-pyridinyl)-, (4aS)- (CA INDEX NAME)

Absolute stereochemistry.

RN 864972-18-9 CAPLUS

CN 1H-Pyrazolo[3,4-g]isoquinoline, 6-[[4-(1,1-dimethylethyl)phenyl]sulfonyl]-4,4a,5,6,7,8-hexahydro-4a-methyl-1-(2-pyridinyl)-, (4aS)- (CA INDEX NAME)

- RN 864972-19-0 CAPLUS
- CN Benzenamine, 4-[[(4aS)-1-(4-fluorophenyl)-1,4,4a,5,7,8-hexahydro-4a-methyl-6H-pyrazolo[3,4-g]isoquinolin-6-yl]sulfonyl]- (CA INDEX NAME)

- RN 864972-20-3 CAPLUS
- CN 1-Propanone, 1-[(4aS)-1-(4-fluorophenyl)-1,4,4a,5,7,8-hexahydro-4a-methyl-6H-pyrazolo[3,4-g]isoquinolin-6-yl]-2,2-dimethyl- (CA INDEX NAME)

Absolute stereochemistry.

- RN 864972-23-6 CAPLUS
- CN 4aH-Pyrazolo[3,4-g]isoquinoline-4a-carboxylic acid, 1-butyl-6-[[4-(1,1-dimethylethyl)phenyl]sulfonyl]-1,4,5,6,7,8-hexahydro-, methyl ester, (4aR)- (CA INDEX NAME)

Absolute stereochemistry.

- RN 864972-24-7 CAPLUS
- CN 4aH-Pyrazolo (3,4-g) isoquinoline-4a-carboxylic acid, 6-[(4-(1,1-dimethylethyl) phenyl] sulfonyl)-1,4,5,6,7,8-hexahydro-1-(1-methylethyl)-, methyl ester, (4aR)- (CA INDEX NAME)

RN 864972-25-8 CAPLUS

CN 4aH-Pyrazolo[3,4-g]isoquinoline-4a-methanol,
6-[[4-(1,1-dimethyl=thyl)phenyl]sulfonyl]-1-(4-fluorophenyl)-1,4,5,6,7,8hexahydro-, (4aR)- (CA INDEX NAME)

Absolute stereochemistry.

RN 864972-26-9 CAPLUS

CN 4aH-Pyrazolo[3,4-g]isoquinoline-4a-methanol,
1-(4-fluorophenyl)-6-[(4-fluorophenyl)sulfonyl]-1,4,5,6,7,8-hexahydro-,
(4aR)- (CA INDEX NAME)

Absolute stereochemistry.

RN 864972-27-0 CAPLUS

CN 4aH-Pyrazolo[3,4-g]isoquinoline-4a-methanol,
1-(4-fluorophenyl)-1,4,5,6,7,8-hexahydro-6-[(4-methylphenyl)sulfonyl]-,
(4aR)- (CA INDEX NAME)

RN 864972-28-1 CAPLUS

CN 4aH-Pyrazolo[3,4-g]isoquinoline-4a-methanol, 1-(4-fluorophenyl)-1,4,5,6,7,8-hexahydro-6-(phenylsulfonyl)-, (4aR)- (CA INDEX NAME)

Absolute stereochemistry.

RN 864972-29-2 CAPLUS

CN 1H-Pyrazolo[3,4-g]isoquinoline, 6-[[4-(1,1-dimethylethyl)phenyl]sulfonyl]-1-(4-fluorophenyl)-4,4a,5,6,7,8-hexahydro-4a-(methoxymethyl)-, (4aR)- (CA INDEX NAME)

Absolute stereochemistry.

RN 864972-30-5 CAPLUS

CN 1H-Pyrazolo[3,4-g]isoquinoline, 6-[[4-(1,1-dimethylethyl)phenyl]sulfonyl]-1-(4-fluorophenyl)-4,4a,5,6,7,8-hexahydro-4a-[(2-methoxyethoxy)methyl]-, (4aR)- (CA INDEX NAME)

Absolute stereochemistry.

RN 864972-31-6 CAPLUS

CN Ethanol, 2-[[(4aR)-1-(4-fluorophenyl)-1,4,5,6,7,8-hexahydro-6-(phenylsulfonyl)-4aH-pyrazolo[3,4-g]isoquinolin-4a-yl]methoxyl- (CA INDEX NAME)

RN 864972-32-7 CAPLUS

CN 1H-Pyrazolo[3,4-g]isoquinoline, 6-[[4-(1,1-dimethylethyl)phenyl]sulfonyl]4a-(ethoxymethyl)-1-(4-fluorophenyl)-4,4a,5,6,7,8-hexahydro-, (4aR)- (CA
NDEX NAME)

Absolute stereochemistry.

- RN 864972-33-8 CAPLUS
- CN 1H-Pyrazolo[3,4-g]isoquinoline, 6-[[4-(1,1-dimethylethyl)phenyl]sulfonyl]-1-(4-fluorophenyl)-4,4a,5,6,7,8-hexahydro-4a-[(3-methoxypropoxy)methyl]-, (4aR)- (CA INDEX NAME)

Absolute stereochemistry.

- RN 864972-34-9 CAPLUS
- CN Propanenitrile, 3-[[(4aR)-6-[[4-(1,1-dimethylethyl)phenyl]sulfonyl]-1-(4-fluorophenyl)-1,4,5,6,7,8-hexahydro-4aH-pyrazolo[3,4-g]isoquinolin-4a-yl]methoxy]- (CA INDEX NAME)

- RN 864972-35-0 CAPLUS
- CN 1H-Pyrazolo[3,4-g]isoquinoline, 6-[[4-(1,1-dimethylethyl)phenyl]sulfonyl]-1-(4-fluorophenyl)-4,4a,5,6,7,8-hexahydro-4a-[[2-(4-dimethyl)]-hoxy|methyl]-, (4aR)- (CA INDEX NAME)

- RN 864972-36-1 CAPLUS
- CN 1H-Pyrazolo[3,4-g]isoquinoline, 6-[[4-(1,1-dimethylethyl)phenyl]sulfonyl]-1-(4-fluorophenyl)-4,4a,5,6,7,8-hexahydro-4a-[[2-1piperidinyl)ethoxy|methyl|-, (4aR)- (CA INDEX NAME)

- RN 864972-37-2 CAPLUS
- CN 1H-Pyrazolo[3,4-g]isoquinoline, 6-[[4-(1,1-dimethylethyl)phenyl]sulfonyl]-

1-(4-fluorophenyl)-4,4a,5,6,7,8-hexahydro-4a-[[2-(1-pyrrolidinyl)ethoxy]methyl]-, (4aR)- (CA INDEX NAME)

Absolute stereochemistry.

RN 864972-38-3 CAPLUS

CN 1H-Pyrazolo[3,4-g]isoquinoline, 1-(4-fluorophenyl)-6-[(4-fluorophenyl)sulfonyl]-4,4a,5,6,7,8-hexahydro-4a-[(2-methoxyethoxy)methyl]-, (4aR)- (CA INDEX NAME)

Absolute stereochemistry.

- RN 864972-39-4 CAPLUS
- CN 1H-Pyrazolo[3,4-g]isoquinoline, 1-(4-fluorophenyl)-6-[(4-fluorophenyl)sulfonyl]-4,4a,5,6,7,8-hexahydro-4a-(methoxymethyl)-, (4aR)-(CA INDEX NAME)

- RN 864972-40-7 CAPLUS
- CN 1H-Pyrazolo[3,4-g]isoquinoline, 1-(4-fluoropheny1)-4,4a,5,6,7,8-hexahydro-4a-(methoxymethy1)-6-[(4-methylpheny1)sulfony1]-, (4aR)- (CA INDEX NAME)

- RN 864972-41-8 CAPLUS
- CN 1H-Pyrazolo[3,4-g]isoquinoline, 1-(4-fluorophenyl)-4,4a,5,6,7,8-hexahydro-4a-[(2-methoxyethoxy)methyl]-6-[(4-methylphenyl)sulfonyl]-, (4aR)- (CA INDEX NAME)

Absolute stereochemistry.

- RN 864972-42-9 CAPLUS
- CN 1H-Pyrazolo[3,4-g]isoquinoline, 1-(4-fluorophenyl)-4,4a,5,6,7,8-hexahydro-4a-[(2-methoxyethoxy)methyl]-6-(phenylsulfonyl)-, (4aR)- (CA INDEX NAME)

Absolute stereochemistry.

- RN 864972-43-0 CAPLUS
- CN 1H-Pyrazolo[3,4-g]isoquinoline, 1-(4-fluorophenyl)-4,4a,5,6,7,8-hexahydro-4a-(methoxymethyl)-6-(phenylsulfonyl)-, (4aR)- (CA INDEX NAME)

RN 864972-44-1 CAPLUS

CN 6H-Pyrazolo[3,4-g]isoquinoline-6-sulfonamide, 1-(4-fluorophenyl)-1,4,4a,5,7,8-hexahydro-4a-[(2-methoxyethoxy)methyl]-N,N-dimethyl-, (4aR)- (CA INDEX NAME)

Absolute stereochemistry.

RN 864972-45-2 CAPLUS

CN 6H-Pyrazolo[3,4-g]isoguinoline-6-sulfonamide, 1-(4-fluorophenyl)-1,4,4a,5,7,8-hexahydro-4a-(methoxymethyl)-N,N-dimethyl-,(4aR)- (CA INDEX NAME)

Absolute stereochemistry.

RN 864972-46-3 CAPLUS

CN 1H-Pyrazolo[3,4-g]isoquinoline, 6-(butylsulfonyl)-1-(4-fluorophenyl)-4,4a,5,6,7,8-hexahydro-4a-[(2-methoxyethoxy)methyl]-, (4aR)- (CA INDEX NAME)

- RN 864972-47-4 CAPLUS
- CN 1H-Pyracolo[3,4-g]isoquinoline, 6-[[4-(1,1-dimethylethyl)phenyl]sulfonyl]-4,4a,5,6,7,8-hexahydro-4a-[(2-methoxyethoxy)methyl]-1-methyl-, (4aR)- (CA INDEX NAME)

- RN 864972-48-5 CAPLUS
- CN 1H-Pyrazolo[3, 4-g]isoquinoline, 1-butyl-6-[[4-(1,1-dimethylethyl)phenyl]sulfonyl]-4, 4a, 5, 6, 7, 8-hexahydro-4a-[(2-methoxyethoxy)methyl]-, (4aR)- (CA INDEX NAME)

Absolute stereochemistry.

- RN 864972-49-6 CAPLUS
- CN 1H-Pyrazolo[3,4-g]isoquinoline, 6-[[4-(1,1-dimethylethyl)phenyl]sulfonyl]-4,4a,5,6,7,8-hexahydro-4a-[(2-methoxyethoxy)methyl]-1-(1-methylethyl)-, (4aR)- (CA INDEX NAME)

- RN 864972-50-9 CAPLUS
- CN 1H-Pyrazolo[3,4-g]isoquinoline, 6-[[4-(1,1-dimethylethyl)phenyl]sulfonyl]-4,4a,5,6,7,8-hexahydro-4a-(methoxymethyl)-1-(1-methylethyl)-, (4aR)- (CA

INDEX NAME)

Absolute stereochemistry.

- RN 864972-51-0 CAPLUS
- CN 1H-Pyrazolo[3,4-g]isoquinoline, 1-buty1-4,4a,5,6,7,8-hexahydro-4a-(methoxymethy1)-6-[(4-methylpheny1)sulfony1]-, (4aR)- (CA INDEX NAME)

Absolute stereochemistry.

- RN 864972-52-1 CAPLUS
- CN 1H-Pyrazolo[3,4-g]isoquinoline, 1-butyl-4,4a,5,6,7,8-hexahydro-4a-[(2-methoxyethoxy)methyl]-6-[(4-methylphenyl)sulfonyl]-, (4aR)- (CA INDEX NAME)

Absolute stereochemistry.

- RN 864972-54-3 CAPLUS
- CN 4aH-Pyrazolo[3,4-g]isoquinoline-4a-methanamine,
  6=[[4-(1,1-dimethyl]-thyl]-phenyl]-ulfonyl]-1-(4-fluorophenyl)-1,4,5,6,7,8hexahydro-N,N-dimethyl-, (4aS)- (CA INDEX NAME)

RN 864972-55-4 CAPLUS

CN 1H-Pyrazolo[3,4-g]isoquinoline, 6-[[4-(1,1-dimethylethyl)phenyl]sulfonyl]-1-(4-fluorophenyl)-4,4a,5,6,7,8-hexahydro-4a-(4-morpholinylmethyl)-,(4a5)- (CA INDEX NAME)

Absolute stereochemistry.

RN 864972-56-5 CAPLUS

CN 1H-Pyrazolo[3,4-g]isoquinoline, 1-(4-fluorophenyl)-4,4a,5,6,7,8-hexahydro-4a-(4-morpholinylmethyl)-6-[[4-(trifluoromethyl)phenyl]sulfonyl]-, (4aS)-(CA INDEX NAME)

Absolute stereochemistry.

RN 864972-57-6 CAPLUS

CN 1H-Pyrazolo[3,4-g]isoquinoline, 6-[(cyclopropylmethyl)sulfonyl]-1-(4-fluorophenyl)-4,4a,5,6,7,8-hexahydro-4a-(4-morpholinylmethyl)-, (4aS)-(CA INDEX NAME)

Absolute stereochemistry.

RN

CN 1H-Pyrazolo[3,4-g]isoquinoline, 6-[[4-(1,1-dimethylethyl)phenyl]sulfonyl]-1-(4-fluorophenyl)-4,4a,5,6,7,8-hexahydro-4a-(1-pyrrolidinylmethyl)-, (4a5)- (CA INBEX NAME)

Absolute stereochemistry.

- RN 864972-59-8 CAPLUS
  - 4 4H-Pyrazolo[3,4-g]isoquinoline-4a-methanamine,
    6-[4-(1,1-dimethylethyl)phenyl]sulfonyl]-N-ethyl-1-(4-fluorophenyl)1,4,5,6,7,8-hexahydro-, (485)- (CA INDEX NAME)

Absolute stereochemistry.

- RN 864972-60-1 CAPLUS
- CN 4aH-Pyrazolo[3,4-g]isoquinoline-4a-methanamine, 6-[[4-(1,1-dimethylethyl)phenyl]sulfonyl]-N,N-ddethyl-1-(4-fluorophenyl)-1.4.5.6,7,8-heashydro-, (4aS)- (CA INDEX NAME)

Absolute stereochemistry.

- RN 864972-61-2 CAPLUS
- CN IH-Pyrazolo[3,4-g]isoquinoline, 6-[[4-{1,1-dimethylethyl]phenyl]sulfonyl]1-(4-fluorophenyl)-4,4a,5,6,7,8-hexahydro-4a-(1-piperidinylmethyl)-,
  (4a5)- (CA INDEX NAME)

- RN 864972-62-3 CAPLUS
- CN 4aH-Pyrazolo[3,4-g]isoquinoline-4a-methanamine,
  6 [[4-(1,1-dimethyl=thyl]phenyl]sulfonyl]-1-(4-fluorophenyl)-1,4,5,6,7,8hexahydro-N-(2-methoxyethyl)-, (4a5)- (CA INDEX NAME)

- RN 864972-63-4 CAPLUS
- CN 1H-Pyrazolo[3, 4-g]isoquinoline, 6-[[4-(1,1-dimethylethyl)phenyl]sulfonyl]-1-(4-fluorophenyl)-4, 4a, 5, 6, 7, 8-hexahydro-4a-[(4-methyl-1piperazinyl)methyl]-, (4a8)- (CA INDEX NAME)

Absolute stereochemistry.

- RN 864972-64-5 CAPLUS
- CN 1,2-Ethanediamine, N2-[[(4aS)-6-[[4-(1,1-dimethylethyl)phenyl]sulfonyl]-1-(4-fluorophenyl)-1,4,5,6,7,8-hexahydro-4aH-pyrazolo[3,4-g]isoquinolin-4ayl]methyl]-N1,N1-dimethyl- (CA INDEX NAME)

- RN 864972-65-6 CAPLUS
- CN 1,2-Ethanediamine, Nl-[[(4aS)-6-[[4-(1,1-dimethylethyl)phenyl]sulfonyl]-1-(4-fluorophenyl)-1,4,5,6,7,8-bexahydro-4aH-pyrazolo[3,4-g]isoquinolin-4a-yl]methyl]-Nl,N2,N2-trimethyl- (CA INDEX NAME)

- RN 864972-66-7 CAPLUS
- CN 1,3-Propanediamine, N3-[(4aS)-6-[(4-(1,1-dimethylethyl)phenyl]sulfonyl]-1-(4-fluorophenyl)-1,4,5,6,7,8-hexahydro-4aH-pyrazolo[3,4-g]isoquinolin-4ayl]methyl]-N1,N1-dimethyl- (CA INDEX NAME)

Absolute stereochemistry.

- RN 864972-67-8 CAPLUS
- CN 1,3=Propanediamine, N1-[[(4aS)-6-[[4-(1,1-dimethylethyl)phenyl]sulfonyl]-1(4-fluorophenyl)-1,4,5,6,7,8-hexahydro-4aH-pyrazolo[3,4-g]isoquinolin-4ayl]methyl]-N1,N3,N3-trimethyl- (CA INDEX NAME)

- RN 864972-68-9 CAPLUS
- CN 4aH-Pyrazolo[3,4-g]isoquinoline-4a-methanamine,
  6 [[4-(1,1-dimethyl=thyl]phenyl]sulfonyl]-1-(4-fluorophenyl)-1,4,5,6,7,8hexahydro-N-(2-methoxyethyl)-N-methyl-, (4a5)- (CA INDEX NAME)

- RN 864972-69-0 CAPLUS
- CN 4aH-Pyrazolo[3,4-g]isoquinoline-4a-methanamine,
  6=[[4-(1,1-dimethyl=thyl)phenyl]sulfonyl]-1-(4-fluorophenyl)-1,4,5,6,7,8hexahydro-N-(1-methyl=thyl)-, (4aS)- (CA INDEX NAME)

Absolute stereochemistry.

- RN 864972-70-3 CAPLUS
- CN 1H-Pyrazolo[3, 4-g]isoquinoline, 4a-(1-azetidinylmethyl)-6-[[4-(1,1-dimethylethyl)phenyl]sulfonyl]-1-(4-fluorophenyl)-4, 4a, 5, 6, 7, 8-hexahydro-, (4aS)- (CA INDEX NAME)

RN 864972-71-4 CAPLUS

CN 4aH-Pyrazolo[3,4-g]isoquinoline-4a-methanamine, 6-[(4-(1,1-dimethyl-thyl)phenyl)sulfonyl]-1-(4-fluorophenyl)-1,4,5,6,7,8hexahydro-N-2-propen-1-yl-, (4aS)- (CA INDEX NAME)

Absolute stereochemistry.

RN 864972-72-5 CAPLUS

CN Ethanol, 2-[[[(4aS)-6-[[4-(1,1-dimethylethyl)phenyl]sulfonyl]-1-(4-fluorophenyl)-1,4,5,6,7,8-hexahydro-4aH-pyrazolo[3,4-g]isoquinolin-4a-yl]methyl]aminol (CA INDEX NAME)

Absolute stereochemistry.

RN 864972-73-6 CAPLUS

CN 4aH-Pyrazolo[3,4-g]isoquinoline-4a-methanamine, 1-(4-fluorophenyl)-1,4,5,6,7,8-hexahydro-N,N-dimethyl-6-[(4-methylphenyl)sulfonyl]-, (4aS)- (CA INDEX NAME)

- RN 864972-74-7 CAPLUS
- CN 1H-Pyrazolo[3,4-g]isoquinoline, 1-(4-fluorophenyl)-4,4a,5,6,7,8-hexahydro-6-[(4-methylphenyl)sulfonyl]-4a-(1-pyrrolidinylmethyl)-, (4aS)- (CA INDEX NAME)

- RN 864972-75-8 CAPLUS
- CN 4aH-Pyrazolo[3,4-g]isoquinoline-4a-methanamine, 1-(4-fluorophenyl)-6-[(4-fluorophenyl)sulfonyl]-1,4,5,6,7,8-hexahydro-N,N-dimethyl-, (4a5) (CA INDEX NAME)

Absolute stereochemistry.

- RN 864972-76-9 CAPLUS
- CN 1H-Pyrazolo[3, 4-g]isoquinoline, 1-(4-fluorophenyl)-6-[(4-fluorophenyl)sulfonyl]-4,4a,5,6,7,8-hexahydro-4a-(1-pyrrolidinylmethyl)-, (4a5)- (CA INDEX NAME)

RN 864972-77-0 CAPLUS

CN 1H-Pyrazolo[3,4-g]isoquinoline, 1-(4-fluorophenyl)-4,4a,5,6,7,8-hexahydro-6-(phenylsulfonyl)-4a-(1-pyrrolidinylmethyl)-, (4aS)- (CA INDEX NAME)

Absolute stereochemistry.

RN 864972-78-1 CAPLUS

CN 4aH-Pyrazolo[3, 4-g]isoquinoline-4a-methanamine, 1-(4-fluorophenyl)-1,4,5,6,7,8-hexahydro-N,N-dimethyl-6-(phenylsulfonyl)-, (4a5)- (CA INDEX NAME)

Absolute stereochemistry.

RN 864972-79-2 CAPLUS

CN 1H-Pyrazolo[3,4-g]isoquinoline, 1-(4-fluorophenyl)-4,4a,5,6,7,8-hexahydro-4a-(4-morpholinylmethyl)-6-(phenylsulfonyl)-, (4aS)- (CA INDEX NAME)

- RN 864972-80-5 CAPLUS
- CN Ethanol, 2-[[[(4aS)-6-[[4-(1,1-dimethylethyl)phenyl]sulfonyl]-1-(4-fluorophenyl)-1,4,5,6,7,8-hexahydro-4aH-pyrazolo[3,4-g]isoquinolin-4a-yl]methyl]methylamino]- (CA INDEX NAME)

- RN 864972-81-6 CAPLUS
- CN 1H-Pyrazolo[3,4-g]isoquinoline, 6-(butylsulfonyl)-1-(4-fluorophenyl)4,4a,5,6,7,8-hexahydro-4a-(4-morpholinylmethyl)-, (4aS)- (CA INDEX NAME)

Absolute stereochemistry.

- RN 864972-82-7 CAPLUS
- CN Benzonitrile, 4-[[(4aS)-1-(4-fluorophenyl)-1,4,4a,5,7,8-hexahydro-4a-(4-morpholinylmethyl)-6H-pyrazolo[3,4-g]isoquinolin-6-yl]sulfonyl]- (CA INDEX NAME)

RN 864972-83-8 CAPLUS

CN 4aH-Pyrazolo[3,4-g]isoquinoline-4a-methanamine, N,N-diethyl-1-(4-fluorophenyl)-1,4,5,6,7,8-hexahydro-6-(phenylsulfonyl)-, (4aS)- (CA INDEX NAME)

Absolute stereochemistry.

RN 864972-84-9 CAPLUS

CN 4AH-Pyrazolo (3,4-g) isoquinoline-4a-methanamine, N,N-diethyl-1-(4-fluorophenyl)-1,4,5,6,7,8-hexahydro-6-[(4-methoxyphenyl) sulfonyl]-, (4aS)- (CA INDEX NAME)

Absolute stereochemistry.

RN 864972-85-0 CAPLUS

CN 1H-Pyrazolo[3,4-g]isoquinoline, 1-(4-fluorophenyl)-4,4a,5,6,7,8-hexahydro-6-(phenylsulfonyl)-4a-(1-piperidinylmethyl)-, (4aS)- (CA INDEX NAME)

- RN 864972-86-1 CAPLUS
- CN 1H-Pyrazolo[3,4-g]isoquinoline, 1-(4-fluorophenyl)-4,4a,5,6,7,8-hexahydro-6-[(4-methoxyphenyl)sulfonyl]-4a-(1-piperidinylmethyl)-, (4aS)- (CA INDEX NAME)

- RN 864972-87-2 CAPLUS
- CN 1H-Pyrazolo[3,4-g]isoquinoline, 1-butyl-4,4a,5,6,7,8-hexahydro-6-[(4-methylphenyl)sulfonyl]-4a-(1-piperidinylmethyl)-, (4aS)- (CA INDEX NAME)

Absolute stereochemistry.

- RN 864972-88-3 CAPLUS
- CN 1H-Pyracolo[3,4-g]isoquinoline, 6-[[4-(1,1-dimethylethyl)phenyl]sulfonyl]-4,4a,5,6,7,8-hexahydro-4a-(1-pyrrolidinylmethyl)-1-(2,2,2-trifluoroethyl)-, (4as)- (CA INDEX NAME)

RN 864972-89-4 CAPLUS

CN 4AH-Pyrazolo[3, 4-g]isoquinoline-4a-methanamine, 1-butyl-6-[[4-(1,1-dimethylethyl)phenyl]sulfonyl]-1,4,5,6,7,8-hexahydro-N,N-dimethyl-, (4a5)- (CA INDEX NAME)

Absolute stereochemistry.

RN 864972-90-7 CAPLUS

CN 1H-Pyrazolo[3,4-g]isoquinoline, 1-butyl-6-[[4-(1,1-dimethylethyl)phenyl]sulfonyl]-4,4a,56,7,8-hexahydro-4a-(1-piperidinylmethyl)-, (4a5)- (CA INDEX NAME)

Absolute stereochemistry.

RN 864972-91-8 CAPLUS

CN 4aH-Pyrazolo[3,4-g]isoquinoline-4a-methanamine, 6-[[4-(1,1-dimethylethyl)phenyl]sulfonyl]-1,4,5,6,7,8-hexahydro-N,Ndimethyl-1-(1-methylethyl)-, (4aS)- (CA INDEX NAME)

Absolute stereochemistry.

RN 864972-92-9 CAPLUS

CN 1H-Pyrazolo[3,4-g]isoquinoline, 6-[[4-(1,1-dimethylethyl)phenyl]sulfonyl]-

4,4a,5,6,7,8-hexahydro-1-(1-methylethyl)-4a-(1-piperidinylmethyl)-, (4aS)-(CA INDEX NAME)

Absolute stereochemistry.

- RN 864972-93-0 CAPLUS
- CN 1H-Pyrazolo[3,4-g]isoquinoline, 1-(4-fluorophenyl)-4,4a,5,6,7,8-hexahydro-6-[(2-methylphenyl)sulfonyl]-4a-(4-morpholinylmethyl)-, (4aS)- (CA INDEX NAME)

Absolute stereochemistry.

- RN 864972-94-1 CAPLUS
- CN 1H-Pyrazolo[3,4-g]isoquinoline, 1-(4-fluorophenyl)-6-[(2-fluorophenyl)sulfonyl]-4,4a,5,6,7,8-hexahydro-4a-(4-morpholinylmethyl)-, (4aS)- (CA INDEX NAME)

Absolute stereochemistry.

- RN 864972-95-2 CAPLUS
- CN 1H-Pyrazolo[3,4-g]isoquinoline, 1-(4-fluoropheny1)-4,4a,5,6,7,8-hexahydro-4a-(4-morpholinylmethy1)-6-(2-pyridinylsulfony1)-, (4aS)- (CA INDEX NAME)

RN 864972-97-4 CAPLUS

CN 4aH-Pyrazolo[3,4-g]isoquinoline-4a-carboxylic acid,
6-[[4-(1,1-dimethyl=thyl]phenyl]sulfonyl]-1-(4-fluorophenyl)1,4,5,6,7,8,8,9-octahydro-, methyl ester, (4aR,8aS)- (CA INDEX NAME)

Absolute stereochemistry.

- RN 864972-99-6 CAPLUS
- CN 1H-Pyrazolo[3,4-g]isoquinoline, 6-[[4-(1,1-dimethylethyl)phenyl]sulfonyl]-1-(4-fluorophenyl)-4,4a,5,6,7,8,8a,9-octahydro-4a-(methoxymethyl)-, (4aR,8aS)- (CA INDEX NAME)

Absolute stereochemistry.

- RN 864973-00-2 CAPLUS
- CN 1R-Pyrazolo[3,4-g]isoquinoline, 6-[[4-(1,1-dimethylethyl)phenyl]sulfonyl]-1-(4-fluorophenyl)-4,4a,5,6,7,8,8a,9-octahydro-4a-[(2methoxyethoxy)methyl]-, (4aR,8aS)- (CA INDEX NAME)

RN 864973-01-3 CAPLUS

CN 1H-Pyrazolo[3,4-g]isoquinoline, 1-(4-fluorophenyl)-4,4a,5,6,7,8,8a,9-octahydro-4a-[(2-methoxyethoxy)methyl]-6-(phenylsulfonyl)-, (4aR,8aS)-(CA INDEX NAME)

Absolute stereochemistry.

RN 864973-02-4 CAPLUS

CN 1H-Pyrazolo[3,4-g]isoquinoline, 1-(4-fluoropheny1)-4,4a,5,6,7,8,8a,9-octahydro-4a-(methoxymethy1)-6-(phenylsulfony1)-, (4aR,8aS)- (CA INDEX NAME)

Absolute stereochemistry.

RN 864973-04-6 CAPLUS

CN 4AH-Pyrazolo[3,4-g]isoquinoline=4a-carboxamide,
6-[[4-(1,1-dimethylethyl)phenyl]sulfonyl]-1-(4-fluorophenyl)-1,4,5,6,7,8hexahydro-N-(phenylmethyl)-, (4aR)- (CA INDEX NAME)

- RN 864973-05-7 CAPLUS
- CN Methanone, [(4aR)-6-[[4-(1,1-dimethylethyl)phenyl]sulfonyl]-1-(4-fiuorophenyl)-1,4,5,6,7,8-hexahydro-4aH-pyrazolo[3,4-g]isoquinolin-4a-yl]-4-morpholinyl- (CA INDEX NAME)

- RN 864973-06-8 CAPLUS
- CN Methanone, [(4aR)-6-[[4-(1,1-dimethylethyl)phenyl]sulfonyl]-1-(4-fluorophenyl)-1,4,5,6,7,8-hexahydro-4aH-pyrazolo[3,4-g]isoquinolin-4a-yl]-1-piperidinyl- (CA INDEX NAME)

Absolute stereochemistry.

- RN 864973-08-0 CAPLUS
- CN Methanone, [(4aR)-6-[[4-(1,1-dimethylethyl)phenyl]sulfonyl]-1-(4-fluorophenyl)-1,4,5,6,7,8-hexahydro-4aH-pyrazolo[3,4-g]isoquinolin-4a-yl]-1-pyrrolidinyl- (CA INDEX NAME)

RN 864973-09-1 CAPLUS

CN 4aH-Pyrazolo[3,4-g]isoquinoline-4a-carboxamide, 6-[[4-(1,1-dimethylethyl)phenyl]sulfonyl]-N-ethyl-1-(4-fluorophenyl)-1,4,5,6,7,8-hexahydro-, (4aR)- (CA INDEX NAME)

Absolute stereochemistry.

RN 864973-11-5 CAPLUS

CN 4AH-Pyrazolo[3,4-g]isoquinoline-4a-carboxamide, 6-[[4-(1,1-dimethylethyl)phenyl]sulfonyl]-1-(4-fluorophenyl)-1,4,5,6,7,8hexahydro-N,N-dimethyl-, (4aR)- (CA INDEX NAME)

Absolute stereochemistry.

RN 864973-12-6 CAPLUS

CN 4aH-Pyrazolo[3,4-g]isoquinoline-4a-methanol, 6-[[4-(1,1-dimethylethyl)phenyl]sulfonyl]-1-(4-fluorophenyl)-1,4,5,6,7,8hexahydro-α-methyl-, (4aR)- (CA INDEX NAME)

RN 864973-13-7 CAPLUS

ON 4aH-Pyrazolo[3,4-g]isoquinoline-4a-methanol, 6-[[4-(1,1-dimethyl-thyl)phanyl]sulfonyl]- $\alpha$ -ethyl-1-(4-fluorophenyl)-1,4,5,6,7,8-hexhydro-, (4aR)- (CA INDEX NAME)

Absolute stereochemistry.

RN 864973-14-8 CAPLUS

CN 4AH-Pyrazolo[3,4-g]isoquinoline-4a-methanol,
6-[[4-(1,1-dimethylethyl)phenyl]sulfonyl]-1-(4-fluorophenyl)-1,4,5,6,7,8hexahydro-α-phenyl-, (4AR)- (CA INDEX NAME)

Absolute stereochemistry.

RN 864973-15-9 CAPLUS

CN Methanone, [(4aR)-6-[[4-(1,1-dimethylethyl)phenyl]sulfonyl]-1-(4-fluorophenyl)-1,4,5,6,7,8-hexahydro-4aH-pyrazolo[3,4-glisoquinolin-4a-yl]phenyl- (CA INDEX NAME)

RN 864973-16-0 CAPLUS

CN 4aH-Pyrazolo[3,4-g]isoquinoline-4a-carboxylic acid, 1-butyl-1,4,5,6,7,8-hexahydro-6-[(4-methylphenyl)sulfonyl]-, methyl ester, (4aR)- (CA INDEX NAME)

Absolute stereochemistry.

RN 864973-17-1 CAPLUS

CN 1H-Pyrazolo[3,4-g]isoquinoline, 1-cyclopentyl-4,4a,5,6,7,8-hexahydro-4a-[(2-methoxyethoxy)methyl]-6-[(4-methylphenyl)sulfonyl]-, (4aR)- (CA INDEX NAME)

Absolute stereochemistry.

RN 864973-23-9 CAPLUS

CN 4AH-Pyrazolo[3,4-g]isoquinoline-4a-ethanamine,
6-[[4-(1,1-dimethylethyl)phenyl]sulfonyl]-1-(4-fluorophenyl)-1,4,5,6,7,8hexahydro-N,N-dimethyl-, (4aR)- (CA INDEX NAME)

- RN 864973-24-0 CAPLUS
- CN 1H-Pyrazolo[3,4-g]isoquinoline, 6-[[4-(1,1-dimethylethyl)phenyl]sulfonyl]-1-(4-fluorophenyl)-4,4a,5,6,7,8-hexahydro-4a-[2-(1-pyrrolidinyl)ethyl]-, (4aR)- (CA INDEX NAME)

- RN 864973-25-1 CAPLUS
- CN 6H-Pyrazolo[3,4-g]isoquinoline-6-carboxylic acid, 1-(4-fluorophenyl)-1,4,4a,5,7,8a,9-octahydro-4a-(4-morpholinylmethyl)-, 1,1-d-imethylethyl ester, (4aS,8aS)- (CA INDEX NAME)

Absolute stereochemistry.

- RN 864973-26-2 CAPLUS
- CN 1H-Pyrazolo[3,4-g]isoquinoline, 6-[[4-(1,1-dimethylethyl)phenyl]sulfonyl]-1-(4-fluorophenyl)-4,4a,5,6,7,8,8a,9-octahydro-4a-(4-morpholinylmethyl)-, (4as,8as)- (CA INDEX NAME)

RN 864973-27-3 CAPLUS

CN 1H-Pyrazolo[3,4-g]isoquinoline, 6-[[4-{1,1-dimethylethyl}]phenyl]sulfonyl]-1-(4-fluorophenyl)-4a-[(4-fluorophenyl)methyl]-4,4a,5,6,7,8-hexahydro-(CA INDEX NAME)

$$\begin{array}{c|c} & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & \\ & & & \\ & &$$

RN 864973-28-4 CAPLUS

CN 1H-Pyrazolo[3,4-g]isoquinoline, 1-(4-fluorophenyl)-4a-[(4-fluorophenyl)methyl]-4,4a,5,6,7,8-hexahydro-6-(phenylsulfonyl)- (CA INDEX NAME)

RN 864973-29-5 CAPLUS

CN 1H-Pyrazolo[3,4-g]isoquinoline, l-(4-fluorophenyl)-4a-[(4-fluorophenyl)methyl]-4,4a,5,6,7,8-hexahydro-6-[(4-methylphenyl)sulfonyl]-(CA INDEX NAME)

RN 864973-30-8 CAPLUS

CN 1H-Pyrazolo[3,4-g]isoquinoline, 1-(4-fluorophenyl)-4a-[(4-

fluorophenyl)methyl]-6-[(4-fluorophenyl)sulfonyl]-4,4a,5,6,7,8-hexahydro-(CA INDEX NAME)

RN 864973-31-9 CAPLUS

CN 1H-Pyrazolo[3,4-g]isoquinoline, 1-(4-fluorophenyl)-4a-[(4-fluorophenyl)methyl]-4,4a,5,6,7,8-hexahydro-6-(methylsulfonyl)- (CA INDEX NAME)

RN 864973-32-0 CAPLUS

CN 1H-Pyrazolo[3,4-g]isoquinoline, 6-(butylsulfonyl)-1-(4-fluorophenyl)-4a-[(4-fluorophenyl)methyl]-4,4a,5,6,7,8-hexahydro- (CA INDEX NAME)

RN 864973-33-1 CAPLUS

CN 1H-Pyrazolo[3,4-g]isoquinoline, 1-(4-fluorophenyl)-4,4a,5,6,7,8-hexahydro-6-[(1-methylethyl)sulfonyl]-4a-(phenylmethyl)- (CA INDEX NAME)

RN 864973-34-2 CAPLUS

CN 1H-Pyrazolo[3,4-g]isoquinoline, 1-(4-fluorophenyl)-4a-[(4fluorophenyl)methyl]-4,4a,5,6,7,8-hexahydro-6-[(1-methyl-1H-imidazol-4yl)sulfonyl]- (CA INDEX NAME)

RN 864973-35-3 CAPLUS

CN 1H-Pyrazolo[3,4-g]isoquinoline, 6-[(3,4-dihydro-4-methyl-2H-1,4-benzoxazin-7-yl)sulfonyl)-1-(4-fluorophenyl)-4a-[(4-fluorophenyl)methyl]-4,4a,5,6,7,8-hexahydro- (CA INDEX NAME)

RN 864973-36-4 CAPLUS

CN 1H-Pyrazolo[3,4-g]isoquinoline, 6-[[6-(1,1-dimethylethyl)-3-pyridinyl]sulfonyl]-1-(4-fluorophenyl)-4a-[(4-fluorophenyl)methyl]-4,4a,5,6,7,8-hexahydro- (CA INDEX NAME)

RN 864973-37-5 CAPLUS

CN 1H-Pyrazolo[3,4-g]isoquinoline, 1-(4-fluorophenyl)-4a-[(4-fluorophenyl)methyl-4,4a,5,6,7,8-hexahydro-6-[(4-(4-morpholinyl)phenyl]sulfonyl- (CA INDEX NAME)

RN 864973-38-6 CAPLUS

CN 1H-Pyrazolo[3,4-g]isoquinoline, 1-(4-fluorophenyl)-4a-[(4-fluorophenyl)methyl]-4,4a,5,6,7,8-hexahydro-6-(4-pyridinylmethyl)- (CA INDEX NAME)

RN 864973-39-7 CAPLUS

CN 1H-Pyrazolo[3,4-g]isoquinoline, 1-(4-fluoropheny1)-4a-[(4-fluoropheny1)methy1]-4,4a,5,6,7,8-hexahydro-6-(3-pyridinylmethy1)- (CA INDEX NAME)

RN 864973-40-0 CAPLUS

CN 1H-Pyrazolo[3,4-g]isoquinoline, 1-(4-fluorophenyl)-4a-[(4-fluorophenyl)methyl]-4,4a,5,6,7,8-hexahydro-6-(2-pyridinylmethyl)- (CA INDEX NAME)

RN 864973-41-1 CAPLUS

CN 1R-Pyrazolo [3, 4-g] isoquinoline, 6-[[6-(1,1-dimethylethyl)-3-pyridinyl]methyl]-1-(4-fluorophenyl)-4a-[(4-fluorophenyl)methyl]-4, 4a, 5, 6, 7, 8-hexahydro- (CA INDEX NAME)

RN 864973-42-2 CAPLUS

CN 1H-Pyrazolo[3,4-g]isoquinoline, 1-(4-fluorophenyl)-4a-[(4-fluorophenyl)methyl]-4,4a,5,6,7,8-hexahydro-6-propyl- (CA INDEX NAME)

- RN 864973-43-3 CAPLUS
- CN 1H-Pyrazolo[3,4-g]isoquinoline, 1-(4-fluorophenyl)-4,4a,5,6,7,8-hexahydro-6-(1H-imidazol-5-ylmethyl)-4a-(phenylmethyl)- (CA INDEX NAME)

- RN 864973-44-4 CAPLUS
- CN 1H-Pyrazolo[3,4-g]isoquinoline, 1-(4-fluorophenyl)-4,4a,5,6,7,8-hexahydro-4a-(phenylmethyl)-6-(4-pyridinylmethyl)- (CA INDEX NAME)

- RN 864973-45-5 CAPLUS
- CN 1H-Pyrazolo[3,4-g]isoquinoline, 1-(4-fluorophenyl)-4a-[(4-fluorophenyl)methyl]-4,4a,5,6,7,8-hexahydro-6-phenyl- (CA INDEX NAME)

- RN 864973-46-6 CAPLUS
- $\begin{array}{ll} \texttt{CN} & \texttt{6H-Pyrazolo[3,4-g]} \\ \texttt{1-(4-fluoropheny1)-4a-[(4-fluoropheny1)methy1]-1,4,4a,5,7,8-hexahydro-N-} \\ \end{array}$

- RN 864973-47-7 CAPLUS
- CN 6H-Pyrazolo[3,4-g]isoquinoline-6-sulfonamide, 1-(4-fluorophenyl)-4a-[(4-fluorophenyl)methyl]-1,4,4a,5,7,8-hexahydro-N-phenyl- (CA INDEX NAME)

- RN 864973-48-8 CAPLUS
- CN 1H-Pyrazolo[3,4-g]isoquinoline, 1-(4-fluoropheny1)-4a-[(4fluoropheny1)methy1]-4,4a,5,6,7,8-hexahydro-6-(4-morpholiny1sulfony1)-(CA INDEX NAME)

- RN 864973-49-9 CAPLUS
- CN 1H-Pyrazolo[3,4-g]isoquinoline, 1-(4-fluorophenyl)-4a-[(4-fluorophenyl)methyl]-4,4a,5,6,7,8-hexahydro-6-[(4-methyl-1-piperazinyl)sulfonyl]- (CA INDEX NAME)

RN 864973-50-2 CAPLUS

CN 1H-Pyrazolo[3,4-g]isoquinoline, 1-(4-fluorophenyl)-4a-[(4-fluorophenyl)methyl]-4,4a,5,6,7,8-hexahydro-6-(1-piperidinylsulfonyl)-(CA INDEX NAME)

RN 864973-51-3 CAPLUS

CN 6H-Pyrazolo[3, 4-g]isoquinoline-6-acetamide, 1-(4-fluorophenyl)-1,4,4a,5,7,8-hexahydro-N,N-dimethyl-4a-(phenylmethyl)-(CA INDEX NAME)

IT 1037050-35-3 1037050-69-3 1037168-91-4 1037183-57-5 1037184-08-9 1037192-71-4 1037201-81-2 1037204-60-6 1037208-30-2 1037210-83-5 1037212-67-1 1037215-77-2 1037217-31-4 1037219-07-0 1037220-44-2 1037221-90-1 1037222-68-6 1037239-93-2 1037292-19-5

RL: RCT (Reactant); RACT (Reactant or reagent)

(preparation of triazacyclopenta[b]naphthalene derivs. as modulators of glucocorticoid receptor)

RN 1037050-35-3 CAPLUS

CN 1H-Pyrazolo[3,4-g]isoquinoline, 4,4a,5,6,7,8-hexahydro-4a-methyl-1-(4-pyridinyl)-, (4aS)- (CA INDEX NAME)

- RN 1037050-69-3 CAPLUS
- CN 1H-Pyrazolo[3,4-g]isoquinoline, 4,4a,5,6,7,8-hexahydro-4a-methyl-1-(2-pyridinyl)-, (4aS)- (CA INDEX NAME)

Absolute stereochemistry.

- RN 1037168-91-4 CAPLUS
- CN 4aH-Pyrazolo[3,4-g]isoquinoline-4a-carboxylic acid,
  1-(4-fluorophenyl)-6-[(4-fluorophenyl)sulfonyl]-1,4,5,6,7,8-hexahydro-,
  methyl ester, (4aR)- (CA INDEX NAME)

Absolute stereochemistry.

- RN 1037183-57-5 CAPLUS
- CN 4AH-Pyrazolo[3,4-g]isoquinoline-4a-carboxylic acid,
  1-(4-fluorophenyl)-1,4,5,6,7,8-hexahydro-6-[(4-methylphenyl)sulfonyl]-,
  methyl ester, (4aR)- (CA INDEX NAME)

RN 1037184-08-9 CAPLUS

CN

4AH-Pyrazolo[3,4-g]isoquinoline-4a-carboxylic acid, 1-(4-fluorophenyl)-1,4,5,6,7,8-hexahydro-6-(phenylsulfonyl)-, methyl ester, (4aR)- (CA INDEX NAME)

Absolute stereochemistry.

RN 1037192-71-4 CAPLUS

CN 6H-Pyracolo[3,4-g]isoguinoline-6-sulfonamide, 1-(4-fluorophenyl)-1,4,4a,5,7,8-hexahydro-4a-(hydroxymethyl)-N,N-dimethyl-,(4aR)- (CA INDEX NAME)

Absolute stereochemistry.

RN 1037201-81-2 CAPLUS

CN 4aH-Pyrazolo[3,4-g]isoquinoline-4a-methanol,
6-(butylsulfonyl)-1-(4-fluorophenyl)-1,4,5,6,7,8-hexahydro-, (4aR)- (CA
INDEX NAME)

RN 1037204-60-6 CAPLUS

CN 4aH-Pyrazolo[3,4-g]isoquinoline-4a-methanol,
6-[[4-(1,1-dimethylethyl)phenyl]sulfonyl]-1,4,5,6,7,8-hexahydro-1-methyl-,
(4aR)- (CA INDEX NAME)

Absolute stereochemistry.

RN 1037208-30-2 CAPLUS

Absolute stereochemistry.

RN 1037210-83-5 CAPLUS

CN 4aH-Pyrazolo[3, 4-g]isoquinoline-4a-carboxaldehyde, 6-[(cyclopropylmethyl)sulfonyl]-1-(4-fluorophenyl)-1,4,5,6,7,8-hexahydro-, (4aS)- (CA INDEX NAME)

RN 1037212-67-1 CAPLUS

CN 4aH-Pyrazolo[3,4-g]isoquinoline-4a-carboxaldehyde,
6-(butylsulfonyl)-1-(4-fluorophenyl)-1,4,5,6,7,8-hexahydro-, (4aS)- (CA
INDEX NAME)

Absolute stereochemistry.

RN 1037215-77-2 CAPLUS

CN Benzonitrile, 4-[[(4aS)-1-(4-fluorophenyl)-4a-formyl-1,4,4a,5,7,8hexahydro-6H-pyrazolo[3,4-g]isoquinolin-6-yl]sulfonyl]- (CA INDEX NAME)

Absolute stereochemistry.

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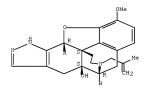
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L7 ANSWER 7 OF 15 CAPLUS COPYRIGHT 2010 ACS on STN

AB Three-dimensional quant. structure-activity relationship (3D-QSAR) models were constructed using comparative mol. field anal. (Co-MFA) on a series of opioid receptor antagonists. To obtain statistically significant and robust Co-MFA models, a sizable data set of naltrindole and naltrexone analogs was assembled by pooling biol. and structural data from independent studies. A process of "leave one data set out", similar to the traditional "leave one out" crossvalidation procedure employed in partial least squares (PLS) anal., was utilized to study the feasibility of pooling data in the present case. These studies indicate that our approach yields statistically significant and highly predictive Co-MFA models from the pooled data set of  $\delta$ ,  $\mu$ , and  $\kappa$  opioid receptor antagonists. All models showed excellent internal predictability and self-consistency: q2 = 0.69/r2 = 0.91 ( $\delta$ ), q2 = 0.67/r2 = 0.92 ( $\mu$ ), and q2 =0.60/r2 = 0.96 (K). The Co-MFA models were further validated using two sep. test sets; one test set was selected randomly from the pooled data set, while the other test set was retrieved from other published sources. The overall excellent agreement between Co-MFA-predicted and exptl, binding affinities for a structurally diverse array of ligands across all three opioid receptor subtypes gives testimony to the superb predictive power of these models. Co-MFA field anal. demonstrated that the variations in binding affinity of opioid antagonists are dominated by steric rather than electrostatic interactions with the three opioid receptor binding sites. The Co-MFA steric-electrostatic contour maps corresponding to the  $\delta$ ,  $\mu$ , and  $\kappa$  opioid receptor subtypes reflected the characteristic similarities and differences in the familiar "message-address" concept of opioid receptor ligands. Structural modifications to increase selectivity for the  $\delta$  over  $\mu$  and  $\kappa$  opioid receptors have been predicted on the basis of the Co-MFA contour maps. The structureactivity relationships (SARs) together with the Co-MFA models should find utility for the rational design of subtype-selective opioid receptor antagonists.

AN 2005:127600 CAPLUS Full-text

- 142:348119 DN
- TΙ 3D-QSAR Comparative Molecular Field Analysis on Opioid Receptor Antagonists: Pooling Data from Different Studies
- AU Peng, Youvi; Keenan, Susan M.; Zhang, Qiang; Kholodovych, Vladyslav; Welsh, William J.
- Department of Pharmacology and the Informatics Institute of UMDNJ, University of Medicine Dentistry of New Jersey-Robert Wood Johnson Medical School (UMDNJ-RWJMS), Piscataway, NJ, 08854, USA
- SO Journal of Medicinal Chemistry (2005), 48(5), 1620-1629 CODEN: JMCMAR; ISSN: 0022-2623
- PB American Chemical Society
- DT Journal
- English LA
- ΤТ 384820-59-1
  - RL: PAC (Pharmacological activity); PRP (Properties); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
  - (3D-QSAR comparative mol. field anal. on opioid receptor antagonists using data from different studies)
- 384820-59-1 CAPLUS RN
- CN 5,10c-(Iminoethano)-10cH-furo[2',3',4',5':4,5]phenanthro[3,2-c]pyrazol-5a(6H)-o1, 4,5,9,9b-tetrahydro-1-methoxy-13-(2-methyl-2-propenyl)-, (5R, 5aS, 9bR, 10cS) - (9CI) (CA INDEX NAME)



- OSC.G 19 THERE ARE 19 CAPLUS RECORDS THAT CITE THIS RECORD (20 CITINGS) RE.CNT 36 THERE ARE 36 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT
- L7 ANSWER 8 OF 15 CAPLUS COPYRIGHT 2010 ACS on STN
- AB Data on opioid abuse liability evaluations of compds. using rhesus monkeys are presented. These data usually involve in vitro evaluation in opioid binding assays, and the compds. may be evaluated for discriminative and reinforcing effects.
- 2003:745070 CAPLUS Full-text AN
- DN 140:264237
- Evaluation of new compounds for opioid activity (2002)
- Woods, J. H.; Ko, M.-C.; Winger, G.; France, C. P.; Traynor, J. R. AU
- CS Departments of Pharmacology and Psychology, University of Michigan, Ann Arbor, MI, USA
- SO NIDA Research Monograph (2003), 183(Problems of Drug Dependence 2002), 170-190
- CODEN: MIDAD4: ISSN: 0361-8595 National Institute on Drug Abuse
- PB
- DT Journal

- LA English
- IT 674347-15-0

RL: ADV (Adverse effect, including toxicity); BSU (Biological study, unclassified); PAC (Pharmacological activity); BIOL (Biological study) (evaluation of new compds. for opioid activity)

- RN 674347-15-0 CAPLUS
- CN 5,10c-(Iminoethano)-10cH-furo[2',3',4',5';4,5]phenanthro[3,2-c]pyrazole-1,5a(6H)-dio1, 4,5,9,9b-tetrahydro-9,13-dimethyl-, dihydrochloride, (5R.5aS.9hR.10cSl- (9CI) (CA INDEX NAME)

- ●2 HC1
- OSC.G 3 THERE ARE 3 CAPLUS RECORDS THAT CITE THIS RECORD (3 CITINGS)
  RE.CNT 13 THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS RECORD
  ALL CITATIONS AVAILABLE IN THE RE FORMAT
- L7 ANSWER 9 OF 15 CAPLUS COPYRIGHT 2010 ACS on STN
- AB The results of a five-year (1997-2002) analgesic and stimulant/depressant testing program, conducted by the Drug Evaluation Committee of the College on Problems of Drug Dependence, are presented. The names of the compds. evaluated, and their mol. structures and a summary of their in vivo and in vitro data are also included.
- AN 2003:745069 CAPLUS Full-text
- DN 140:264236
- TI Biological evaluation of compounds for their physical dependence potential and abuse liability. XXVI. Drug Evaluation Committee of the College on Problems of Drug Dependence (2002)
- AU Coop, A.
- CS Department of Pharmaceutical Sciences, University of Maryland School of Pharmacy, Baltimore, MD, USA
- SO NIDA Research Monograph (2003), 183(Problems of Drug Dependence 2002), 152-169
  - CODEN: MIDAD4; ISSN: 0361-8595
- PB National Institute on Drug Abuse
- DT Journal LA English
- LA English
- IT 674347-15-0
  - RL: ADV (Adverse effect, including toxicity); BSU (Biological study, unclassified); PAC (Pharmacological activity); BIOL (Biological study) (biol. evaluation of compds. for their phys. dependence potential and abuse liability)
- RN 674347-15-0 CAPLUS
- CN 5,10c-(Iminoethano)-10cH-furo[2',3',4',5':4,5]phenanthro[3,2-c]pyrazole-

1,5a(6H)-diol, 4,5,9,9b-tetrahydro-9,13-dimethyl-, dihydrochloride, (5R,5aS,9bR,10cS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

●2 HC1

# RE.CNT 11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

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chain nodes : 14 ring nodes :

chain bonds : 7-14

ring bonds :

1-2 1-5 1-9 2-3 3-4 4-5 5-6 6-7 7-8 7-10 8-9 8-13 10-11 11-12 12-13 15-16 15-20 16-17 17-18 18-19 19-20 21-22 21-26 22-23 23-24 24-25 25-26 exact/norm bonds :

normalized bonds : 21-22 21-26 22-23 23-24 24-25 25-26

G1:C,N

Match level: 1:1:CLASS 2:CLASS 3:CLASS 4:CLASS 5:CLASS 6:CLASS 7:CLASS 8:CLASS 9:CLASS 10:CLASS 11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS 19:CLASS 20:CLASS 21:CLASS 22:CLASS 23:CLASS 24:CLASS 25:CLASS 26:CLASS 25:CLASS 25:CLASS 25:CLASS 26:CLASS 25:CLASS 25:CLA

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L4 2 L3

- L4 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2010 ACS on STN
- AB Addn. of the 4-fluorophenylpyrazole group to the previously described 2-azadecalin glucocorticoid receptor (GR) antagonist 1 resulted in significantly enhanced functional activity. SAR of the bridgehead substituent indicated that whereas groups as small as Me afforded high GR binding, GR functional activity was enhanced by larger groups such as benzyl, substituted ethers, and aminoalkyl derivs. GR antagonists with binding and functional activity comparable to mifepristone were discovered (e.g., 52: GR binding KO 7 nM; GR reporter gene functional Ki 0.6 nM) and found to be highly selective over other steroid receptors. Analogs 43 and 45 had >50% oral bioavailability in the dog.
- AN 2008:232071 CAPLUS Full-text
- DN 148:440269
- TI 1H-Pyrazolo[3,4-g]hexahydro-isoquinolines as selective glucocorticoid receptor antagonists with high functional activity
- AU Clark, Robin D.; Ray, Nicholas C.; Williams, Karen; Blaney, Paul; Ward, Stuart; Crackett, Peter H.; Hurley, Christopher; Dyke, Hazel J.; Clark, David E.; Lockey, Peter; Devos, Rene; Wong, Melanie; Porres, Soraya S.; Bright, Colin P.; Jenkins, Robert E.; Belanoff, Joseph
- CS Corcept Therapeutics, Menlo Park, CA, 94025, USA
- SO Bioorganic & Medicinal Chemistry Letters (2008), 18(4), 1312-1317 CODEN: BMCLE8: ISSN: 0960-894X
- PB Elsevier Ltd.
- DT Journal
- LA English
- OS CASREACT 148:440269
- IT 864972-01-1P

RL: DMA (Drug mechanism of action); PAC (Pharmacological activity); PKT (Pharmacokinetics); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(1H-pyrazolo[3,4-g]hexahydro-isoquinolines as selective glucocorticoid receptor antagonists)

- RN 864972-02-1 CAPLUS
- CN 1H-Pyrazolo[3,4-g]isoquinoline, 6-[[4-(1,1-dimethylethyl)phenyl]sulfonyl]-1-(4-fluorophenyl)-4,4a,5,6,7,8-hexahydro-4a-methyl-, (4a5)- (CA INDEX NAME)

- OSC.G 5 THERE ARE 5 CAPLUS RECORDS THAT CITE THIS RECORD (5 CITINGS)
  RE.CNT 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD
  ALL CITATIONS AVAILABLE IN THE RE FORMAT
- L4 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2010 ACS on STN

$$\underbrace{ \begin{bmatrix} L^{1} - R^{1} \\ A \end{bmatrix} }_{L^{2} - R^{2}}$$

Title compds. I [L1 and L2 independently = a bond, O, S, etc.; A = AB (un) substituted 5-6 membered heterocycloalkyl or heteroaryl; R1 = H, (un) substituted alkyl, heteroalkyl, etc.; R2 = (un) substituted alkyl, heteroalkyl, cycloalkyl, etc.] and their pharmaceutically acceptable salts, are prepared and disclosed as modulators of qlucocorticoid receptor. Thus, II was prepared by cyclization of (S)-8a-benzyl-2-(4-tert-butyl-benzenesulfonyl)-7-[1-hydroxy-meth-(Z)- ylidene]-1,3,4,7,8,8a-hexahydro-2H-isoquinolin-6-one (preparation given) with hydrazine hydrate. The activity of I was evaluated in glucocorticoid receptor binding assay and it was revealed that selected compds. of the invention displayed IC50 values in the range of 10 up to 100 nm and others below 10 nM. Pharmaceutical compns. comprising I are disclosed. AN

2005:1021750 CAPLUS Full-text

DN 143:306309

- Preparation of triazacyclopenta[b]naphthalene derivatives as modulators of ΤI glucocorticoid receptor
- IN Clark, Robin D.; Ray, Nicholas C.; Blaney, Paul M.; Hurley, Christopher A.; Williams, Karen
- PA Corcept Therapeutics, Inc., USA
- PCT Int. Appl., 160 pp. SO

CODEN: PIXXD2

DT Patent

LA English

FAN.CNT 1

		CITT																		
		PA:	ENT :	NO.			KIN	D	DATE			APPL	ICAT	ION I	.00		D	ATE		
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PI WO 2005087769					A1 20050922			WO 2005-US8049				20050309								
			W:	ΑE,	AG,	AL,	AM,	AT,	AU,	AZ,	BA,	BB,	BG,	BR,	BW,	BY,	BZ,	CA,	CH,	
				CN,	CO,	CR,	CU,	CZ,	DE,	DK,	DM,	DZ,	EC,	EE,	EG,	ES,	FI,	GB,	GD,	
				GE,	GH,	GM,	HR,	HU,	ID,	IL,	IN,	IS,	JP,	KE,	KG,	KP,	KR,	KZ,	LC,	
				LK,	LR,	LS,	LT,	LU,	LV,	MA,	MD,	MG,	MK,	MN,	MW,	MX,	MZ,	NA,	NI,	
				NO,	NZ,	OM,	PG,	PH,	PL,	PT,	RO,	RU,	SC,	SD,	SE,	SG,	SK,	SL,	SM,	
				SY,	TJ,	TM,	TN,	TR,	TT,	TZ,	UA,	UG,	US,	UZ,	VC,	VN,	YU,	ZA,	ZM,	ZW
			RW:	BW,	GH,	GM,	KE,	LS,	MW,	MZ,	NA,	SD,	SL,	SZ,	TZ,	UG,	ZM,	ZW,	AM,	
				AZ,	BY,	KG,	KZ,	MD,	RU,	TJ,	TM,	AT,	BE,	BG,	CH,	CY,	CZ,	DE,	DK,	
				EE,	ES,	FI,	FR,	GB,	GR,	HU,	IE,	IS,	IT,	LT,	LU,	MC,	NL,	PL,	PT,	
				RO,	SE,	SI,	SK,	TR,	BF,	BJ,	CF,	CG,	CI,	CM,	GA,	GN,	GQ,	GW,	ML,	
				MR,	NE,	SN,	TD,	TG												
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	CA	2558899			A1	2	2005	0922		CA	200	05-2	2558	899		2	0050	309
	EP	1735308			A1	2	2006	1227	1	EP	200	05-	7252	95		2	0050	309
	EP	1735308			В1	2	2008	0910										
		R: AT	BE,	BG,	CH,	CY,	CZ,	DE,	DK,	EE	, I	ES,	FI,	FR,	GB,	GR,	HU,	IE,
		IS	IT,	LI,	LT,	LU,	MC,	NL,	PL,	PT	, 1	RO,	SE,	SI,	SK,	TR		
	CN	1010273	)1		A	2	2007	0829		CN	200	05-1	3001	1481		2	0050	309
JP 2007528417				T	2	JP 2007-503030							20050309					
AT 407934			T	20080915			AT 2005-725295						20050309					
	PT	1735308			E	2	2008	1202	1	PΤ	200	05-	7252	95		2	0050	309
	ES	2313317			Т3	2	2009	0301	1	ES	200	05-	7252	95		2	0050	309
	za	2006008	306		A	2	2009	0225		ZA	200	06-8	3306			2	0061	005
	KR	2007029	584		A	2	2007	0314	1	KR	200	06-	7209	88		2	0061	009
	IN	2006CN0	3745		A	2	2007	0615		IN	200	06-0	N37	45		2	0061	009
	US	2007028	1928		A1	2	2007	1206	1	US	200	07-	5918	84		2	0070	507
	HK	1104813			A1	2	2009	0403	1	HK	200	07-:	1069	03		2	0070	627
PRAI	US	2004-55	1836P		P	2	2004	0309										
	WO	2005-US	3049		W	2	2005	0309										

ASSIGNMENT HISTORY FOR US PATENT AVAILABLE IN LSUS DISPLAY FORMAT CASREACT 143:306309; MARPAT 143:306309

864972-22-5P IT

RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(preparation of triazacyclopenta[b]naphthalene derivs. as modulators of glucocorticoid receptor)

864972-22-5 CAPLUS RN

4aH-Pyrazolo[3,4-g]isoquinoline-4a-carboxylic acid, CN

6-[[4-(1,1-dimethylethyl)phenyl]sulfonyl]-1-(4-fluorophenyl)-1,4,5,6,7,8hexahydro-, methyl ester, (4aR)- (CA INDEX NAME)

Absolute stereochemistry.

- OSC.G THERE ARE 3 CAPLUS RECORDS THAT CITE THIS RECORD (4 CITINGS) RE.CNT 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT
- => file registry
- on property searching in REGISTRY, refer to:

http://www.cas.org/support/stngen/stndoc/properties.html

Uploading C:\Program Files\Stnexp\Queries\10591884.str

chain nodes:
14
ring nodes:
1 2 3 4 5 6 7 8 9 10 11 12 13
chain bonds:

7-14 ring bonds :

G1:C,N

Match level: 1:CLASS 3:CLASS 4:CLASS 5:CLASS 6:CLASS 7:CLASS 8:CLASS 9:CLASS 10:CLASS 11:CLASS 12:CLASS 13:CLASS 14:CLASS

### L5 STRUCTURE UPLOADED

=> d 15 L5 HAS NO ANSWERS L5 STR



Structure attributes must be viewed using STN Express query preparation.

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SAMPLE SEARCH INITIATED 16:09:26 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 474 TO ITERATE
100.0% PROCESSED
                 474 ITERATIONS
                                                             10 ANSWERS
SEARCH TIME: 00.00.01
FULL FILE PROJECTIONS: ONLINE **COMPLETE**
                      BATCH **COMPLETE**
PROJECTED ITERATIONS:
                     8174 TO 10786
PROJECTED ANSWERS:
                             11 TO
                                      389
1.6
           10 SEA SSS SAM L5
=> s 15 full
FULL SEARCH INITIATED 16:09:34 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 10016 TO ITERATE
100.0% PROCESSED 10016 ITERATIONS
                                                           200 ANSWERS
SEARCH TIME: 00.00.01
L7 200 SEA SSS FUL L5
=> file caplus
http://www.cas.org/legal/infopolicy.html
This file contains CAS Registry Numbers for easy and accurate
substance identification.
=> s 17
1.8
          2 L7
=> d his
     (FILE 'HOME' ENTERED AT 16:06:10 ON 14 JUL 2010)
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L1
              STRUCTURE UPLOADED
L2
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L3
           163 S L1 FUL
   FILE 'CAPLUS' ENTERED AT 16:06:58 ON 14 JUL 2010
L4
            2 S L3
    FILE 'REGISTRY' ENTERED AT 16:09:03 ON 14 JUL 2010
1.5
              STRUCTURE UPLOADED
L6
            10 S L5
           200 S L5 FULL
L7
   FILE 'CAPLUS' ENTERED AT 16:09:38 ON 14 JUL 2010
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=> file stnguide FILE CONTAINS CURRENT INFORMATION. LAST RELOADED: Jul 9, 2010 (20100709/UP).

2 S L7

0 L8 NOT L4

L8

L9

=> s 18 not 14